Corporate Investment and Financing Dynamics

Dirk Hackbarth* Dongming Sun†

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Abstract

This paper studies the behavior of leverage ratios in a dynamic trade-off model with real frictions. Firms underutilize debt when financing investment to retain financial flexibility. Underutilization of debt persists even when firms exercise their last investment options, and it is more (less) severe for more back-loaded (front-loaded) investment opportunities. Thus, leverage dynamics crucially hinge upon the structure of the investment process and otherwise identical firms appear to have significantly different target leverage ratios. Structural estimation of key parameters reveals that simulated model moments can match data moments. We obtain capital structure regression results in line with the empirical evidence, and explain the empirical puzzle that average leverage ratios are path-dependent and persistent for extended periods of time.

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*Department of Finance, Boston University, 595 Commonwealth Avenue, Boston, MA 02215, United States.

†Department of Finance, University of Illinois, 515 East Gregory Drive, Champaign IL 61820, United States.

1 Introduction

Since Modigliani and Miller (1958), economists have relaxed many of their assumptions to understand the observed behavior of leverage ratios. Arguably, the trade-off theory has emerged as one of the leading paradigms, even though it has often been challenged by empirical tests that appear to favor other theories or suggest taxes are not that important. Therefore, there is still no consensus in the literature. Moreover, none of the extant theories address jointly the following questions in a parsimonious and simple framework: (1) why firms tend to use debt financing so conservatively, (2) whether there is indeed a target leverage ratio and partial adjustment towards it, (3) why the leverage-growth relation is negative and (4) why average leverage paths persist for over two decades.

To answer these questions, we analyze a framework in the spirit of Hackbarth and Mauer (2012), in which investment and financing decisions are endogenously determined. In particular, we develop two versions of a dynamic model While the multi-stage model features two sequentially exercisable investment options, the single-stage model has only one investment option. The single-stage model serves as a benchmark to gauge investment-financing interactions in the otherwise identical multi-stage model. In both versions, the capital expenditure can be financed by a mixture of equity and debt. This mixture not only trades off tax benefits of debt against bankruptcy costs (triggered by an endogenous default decision) but also recognizes financial flexibility in the multi-stage model.

The solution of the model generates a rich set of testable predictions that link the behavior of a firm's leverage ratios to its investment opportunities. First, dynamic financing-investment interactions between investment stages lead to an "intertemporal effect" in the multi-stage model: reaping investment benefits sooner by issuing more debt in the first stage to fund the investment cost reduces financial flexibility for funding more of the investment cost with debt in the second stage. In comparison to the single-stage model, firms underutilize debt in the multi-stage model when financing investment the first time to retain financial flexibility. In fact, underutilization of debt persists when firms mature (i.e. exercise their last investment options), and it is more (less) severe for more back-loaded (front-loaded) investment opportunities. It is worth noting that leverage does not vary with investment in the single-stage model. Only in the multi-stage model leverage dynamics crucially hinge upon the structure of the investment process and otherwise identical firms appear to have significantly different target leverage ratios.[1]

[1] Consistent with these observations, capital structure tests that recognize investment emerged relatively recently (e.g. Harford et al. (2009), Denis and McKeon (2012), Eckbo and Kisser (2015), or Elsas et al. (2015)).

Second, optimizing behavior by firms in a dynamic trade-off model with investment generates without any other frictions (e.g. agency conflicts or transaction costs) a significant fraction of low and zero leverage firms and also path-dependent, persistent leverage ratios. Our analysis shows how incentives to retain financial flexibility in the first stage crucially depend on the structure of the investment process. Given the wide range of optimal target leverage ratios, the model suggests that leverage ratios can greatly vary depending on how the firm grows assets-in-place by exercising its real options. Third, structural models without dynamic financing-investment interactions (1) overestimate target leverage ratios, and (2) can be misleading in that they imply a fixed target leverage ratio that is largely taken to be exogenous to the investment process. It thus seems difficult to determine target leverage in the conventional sense. This also suggests that there is no meaningful measurement of partial adjustment towards target leverage (as e.g. in Flannery and Rangan (2006)) without recognizing the structure of the investment process.[2]

To test the model's ability to match observed outcomes, we estimate key model parameters via Simulated Method of Moments (SMM).[3] Intuitively, SMM finds the set of parameters, which minimizes the difference of the simulated model moments and the data moments from COMPUSTAT's annual tapes for the period of 1965 to 2009. We then split the full sample into low, medium, and high market-to-book (or Q) subsamples, and employ SMM also to fit the four parameters for each subsample. We split the sample based on Q to proxy for investment opportunities. Low Q firms tend to have fewer investment opportunities, whereas high Q firms tend to have more investment opportunities. Therefore, the relative value of Q is informative about the structure of the investment process in the real data. Our estimation results reveal that high Q firms have the most back-loaded investment processes, and low Q firms have the most front-loaded ones.

Graham (2000) reports that firms, even stable and profitable, use less debt than predicted by the static view of the tax benefits of debt. Two out of five firms have an average leverage ratio of less than 20%, and the median firm uses only 31.4% leverage over the 1965 to 2000 period, which implies a "low leverage puzzle." In addition, Strebulaev and Yang (2012) find that on average 10% of firms have zero leverage and almost 22% firms have less than 5% quasi-market leverage, which represents a "zero leverage puzzle." We emphasize the importance of real frictions in a dynamic

[2] This is in line with recent research (e.g. Hovakimian and Li (2012)), which argues partial adjustment regressions are ill-suited for determining the performance of dynamic trade-off models. In addition, Denis (2012) concludes that traditional models do a remarkably poor job of explaining the dynamics of observed capital structures.

[3] A careful calibration, as e.g. in Strebulaev (2007), would suffice for our purposes, as we estimate four parameters. A benefit of SMM, is, however, that it informs us about the role of taxes and the variation in investment characteristics.

trade-off model and thereby provide an economically meaningful mechanism for why firms tend to use debt financing so conservatively. Based on the structural estimation results for the full sample, the simulated economies feature a significant fraction of low (and zero) leverage firms. Moreover, in contrast to much higher point estimates in prior studies, we report, on average, 20% leverage in dynamics (i.e. for all firms) and 19% at investment points (i.e. for investing firms).

In addition, we perform capital structure regressions on simulated data and show that the model can replicate stylized facts established by empirical research. In the spirit of Strebulaev (2007), simulation of the multi-stage model of corporate investment and financing dynamics reinforces the need to differentiate investment points from other data points when interpreting coefficient estimates for market-to-book or profitability in a dynamic world. Consistent with Frank and Goyal (2009) and others, we find leverage is negatively related to the risk of cash flows, the cost of bankruptcy, and market-to-book, but positively related the size of the firm and the tax rate.

Finally, we document that real frictions in a dynamic model can produce average leverage paths that closely resemble the ones in the data (e.g. Lemmon, Roberts and Zender (2008)).[4] That is, endogenous investment and financing decisions in a dynamic model can largely explain the otherwise puzzling patterns that, despite of some convergence, average leverage ratios across portfolios are fairly stable over time for both types of sorts (i.e. actual and unexpected leverage) performed by these authors.[5] To do so, we extend the multi-stage model to randomly imposed initial variation in leverage. If model firms are "born" with high (low) leverage ratios at the beginning, then they maintain their relatively high (low) levels for over two decades (despite of the fact that leverage ratios converge somewhat to more moderate levels over time). This result illustrates that corporations, which know the structure of their investment processes, take it into account and make decisions on debt usage accordingly. This leads to fairly stable leverage ratios, and serves in the simulations as an important, unobserved determinant of the permanent component of leverage.

Our paper contributes to the growing literature that extends Leland (1994) to interactions between investment and financing decisions (see e.g. Morellec and Schuerhoff (2011), Hackbarth and Mauer (2012), or Sundaresan, Wang, and Yang (2015)). To the best of our knowledge, however, this paper is the first that derives the capital structure implications of the structure of the investment

[4] Eckbo and Kisser (2015) find that much of the leverage ratio instability reported by DeAngelo and Roll (2015) is driven by high-frequency net-debt issuers, whose real frictions might be low in spite of their high investment rates.

[5] In this part of the paper, we employ the structural estimation results for the three subsamples to introduce industry variation, so sorting on "unexpected leverage" defined as the residuals from a cross-sectional regression of leverage on firm characteristics and industry indicator variables is different from sorting on actual leverage.

process (cf. the intertemporal effect) in a multi-stage model of jointly optimal financing and investment decisions and that reports structural parameter estimates for this class of models.[6] This allows us to generate additional insights for capital structure research and to better understand (heretofore puzzling) empirical regularities by studying simulated data panel sets with real (i.e. investment) frictions, such as, capital structure persistence and profitability-leverage (or Q-leverage) dynamics.

Furthermore, our paper relates to dynamic capital structure models without investment that rely on transaction costs (see e.g. Fischer, Heinkel, and Zechner (1989), Leary and Roberts (2005), and Strebulaev (2007)). While transaction costs are largely constant over time, time-variation of real frictions is a realistic and useful modeling tool, because some firms have more front-loaded investment opportunities whereas others have more back-loaded ones, but all firms exhaust their investment opportunities over time. Like us, Hennessy and Whited (2005, 2007) analyze a dynamic trade-off model with investment and perform structural estimation. While we focus on the structure of the investment process in a real options model with multiple issues of risky debt, they largely focus on the role of tax regimes in a different class of models. More recently, Tserlukevich (2008) also invokes real fictions to produce gradual and lumpy leverage adjustments in the absence of financial frictions. Two key differences are that there is no intertemporal effect in his model and that leverage ratios produced by his model are much higher than ours.[7] In addition, we perform various tests of the model's ability to explain observed leverage patterns (i.e. structural estimation, capital structure regressions, and leverage portfolio sorts). DeAngelo, DeAngelo, and Whited (2011) study transitory debt that arises due to unexpected (positive) shocks to investment opportunities whose properties are uncertain as of time zero. Our model firm optimizes at the beginning knowing the structure of the investment process, so there is no role for transitory debt. Consistent with our findings, Li, Whited and Wu (2015) show that the value of preserving financial flexibility is important even in an environment with limited enforcement where collateral constraints matter more for capital structure than tax benefits. In contrast, our estimates suggest that sizable tax benefits can coexist with financial flexibility.

The paper is organized as follows. Section 2 presents and solves the model. Section 3 studies the intertemporal effect. Section 4 estimates structural parameters using SMM. Section 5 first describes simulated panel data sets on which we then perform capital structure tests. Section 6 concludes.

[6] See Strebulaev and Whited (2012) for review of structural models and structural estimation in corporate finance.

[7] He assumes free leverage adjustments in a world with taxes but without bankruptcy costs. Unlike our setup, debt is risk-free in his setup and rebalanced continuously. Hence leverage ratios are high relative to empirical estimates.

2 Model

This section provides a simple framework to study the effects of financial flexibility. In particular, we develop two versions of a dynamic model with endogenous financing and investment decisions, where capital expenditures are financed by a mixture of equity and debt. While the multi-stage model features two sequentially exercisable investment options, the single-stage model has only one investment option. The single-stage model serves as a benchmark to gauge interactions between corporate investment and financing decisions in the otherwise identical multi-stage model.

2.1 Setup

We consider a partial equilibrium model of corporate investment and financing dynamics. Time t is continuous and uncertainty is modeled by a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Corporate assets generate a continuous stream of cash flows, X_t, which evolve for $t > 0$ according to a geometric Brownian motion with drift μ, volatility σ, and initial value initial cash flow $X_0 > 0$ at time $t = 0$. Corporate taxes are paid on cash flows at a constant rate τ based on full loss offset provisions. Agents are risk-neutral and discount cash flows at a constant interest rate $r > \mu$.

At time $t = 0$, the firm has no assets-in-place and a two-stage project, i.e. a compound option in that the implementation of the second stage investment is contingent upon the completion of the first stage. The two constants Π_1 and Π_2 represent the scales of the two investment options (or, more broadly, the structure of the investment process). Suppressing time dependence of cash flows, $\Pi_i X$ is the cash flow from investing in stage $i = 1, 2$, which requires a capital expenditure, F_i.

The investment cost, F_i, can be financed with a mix of debt and equity. We assume that debt has an infinite maturity and denote the coupon rate on debt issued in stage i by C_i.[8] The optimal time to invest is the one that maximizes the market value of equity. The optimal time to default on debt coupon payments is also endogenously determined (i.e. maximizes equity value). In the event of default, equityholders receive nothing and debtholders assume ownership of the firm's assets net of bankruptcy costs. Bankruptcy costs include the loss of interest tax shields, the loss of the second-stage option (if it has not been exercised), and the fraction α of the value of assets-in-place. The endogenous investment thresholds and default thresholds in stage i are X_{Si} and X_{Di} for $i = 1, 2$.[9]

[8] Elsas, Flannery, and Garfinkel (2015) document that large investments are mostly externally financed and, in particular that firms issue debt to move toward target debt ratios. The reliance on consol bonds simplifies the analysis substantially but does not alter the economic insights.

[9] See Appendix A and Section 5.3 for a multi-stage model extended to have also an initial debt coupon C_0.

At time $t = 0$, equityholders wait to exercise the first investment option, which is triggered when cash flows rise to the investment threshold $X_{S1} \in (X_0, \infty)$ for the first time from below. We denote this waiting period "stage 0" and call the firm in this stage a "juvenile" firm. When the first option is exercised, the firm issues debt D_1 and equity E_1 to finance the fixed investment cost F_1. Then the firm enters "stage 1" and becomes an "adolescent" firm.

In stage 1, the firm has assets-in-place, another investment option, and a default option because of D_1. If cash flows decline to the default threshold $X_{D1} \in (0, X_{S1})$ before reaching the second investment threshold $X_{S2} \in (X_{S1}, \infty)$, equityholders default. On the other hand, if cash flows reach the investment threshold X_{S2} before decreasing to X_{D1}, equityholders exercise the second option and finance the investment cost F_2 with a mix of debt, D_{22}, and equity, E_2. We assume that D_{22} has the same seniority as D_1 whose value is denoted as D_{21} in the second stage. The firm then enters "stage 2" and becomes a "mature" firm.

In stage 2, the firm has assets-in-place, no further investment options, and a default option because of D_{21} and D_{22}. Equityholders default when X touches the default threshold $X_{D2} \in (0, X_{S2})$ for the first time from above. Finally, we assume that there are no conflicts of interest and the debt coupons, C_1 and C_2, maximize equity value at time 0, E_0. Table 1 provides a notational key.

[Insert Table 1 Here.]

To identify dynamic interactions of endogenous investment and financing decisions, we use a single-stage model as a benchmark. This single-stage model is a truncated version of the multi-stage model in that there is no intermediate stage 1. In stage 0, the juvenile firm has no asset-in-place and no debt. It makes one investment of scale Π when X touches the investment threshold X_S from below for the first time, and then becomes a mature firm (i.e. enters stage 2). The capital expenditure, F, is funded by a mixture of debt and equity, where C denotes the coupon of the firm's debt issue.

2.2 Solution of the Multi-Stage Model

Using backward induction, we obtain values of debt and equity in each stage and then pin down the endogenous investment and default thresholds via smooth-pasting conditions.

2.2.1 Mature Firm (Stage 2)

In the second stage, both investment options have been converted into assets-in-place. The second debt issue, D_{22}, which partially finances the investment cost, F_2, and the first debt issue, D_{21}, offer

tax savings but give rise to a default decision (or threshold X_{D2}). Following standard arguments, the debt issue's value, $D_{2i}(X, C_1, C_2)$, $i = 1, 2$, has for $X \geq X_{D2}$ a solution of the form:[10]

$$D_{2i}(X, C_1, C_2) \;=\; A_{1i}X^a + A_{2i}X^z + \frac{C_i}{r}, \tag{1}$$

where the two exponents $a < 0$ and $z > 1$ are the negative and positive roots of the quadratic equation $y(y-1)\frac{1}{2}\sigma^2 + y\mu - r = 0$. The constants A_{1i} and A_{2i} solve the following boundary conditions. When $X \uparrow \infty$, debt becomes risk-free and its value equals the present value of a perpetuity: $D_{2i}(\infty, C_1, C_2) = \frac{C_i}{r}$. On the other hand, when X declines to X_{D2}, equityholders default and the owners of D_{2i} get a proportion of the liquidation value based on the coupon C_i for $i = 1, 2$:[11]

$$D_{2i}(X_{D2}, C_1, C_2) \;=\; \frac{C_i}{C_1 + C_2}\frac{(1-\alpha)(1-\tau)(\Pi_1 + \Pi_2)X_{D2}}{r - \mu}, \;\; i = 1, 2. \tag{2}$$

Equity value $E_2(X, C_1, C_2)$, on the other hand, has for $X \geq X_{D2}$ a solution of the form:

$$E_2(X, C_1, C_2) \;=\; B_1X^a + B_2X^z + (1-\tau)\Big(\frac{(\Pi_1 + \Pi_2)X}{r - \mu} - \frac{(C_1 + C_2)}{r}\Big), \tag{3}$$

where the constants B_1 and B_2 satisfy the following boundary conditions:

$$E_2(X_{D2}, C_1, C_2) \;=\; 0, \tag{4}$$

$$E_2(\infty, C_1, C_2) \;=\; (1-\tau)\Big(\frac{(\Pi_1 + \Pi_2)X}{r - \mu} - \frac{(C_1 + C_2)}{r}\Big). \tag{5}$$

Simple algebra yields the value of the two debt issues for $X \geq X_{D2}$:

$$D_{2i}(X, C_1, C_2) \;=\; \frac{C_i}{r}\Big(1 - (\frac{X}{X_{D2}})^a\Big) + \frac{C_i}{C_1 + C_2}\frac{(1-\alpha)(1-\tau)(\Pi_1 + \Pi_2)X_{D2}}{r - \mu}(\frac{X}{X_{D2}})^a, \tag{6}$$

with $i = 1, 2$, and also the value of equity for $X \geq X_{D2}$:

$$E_2(X, C_1, C_2) \;=\; (1-\tau)\Big(\frac{(\Pi_1 + \Pi_2)X}{r - \mu} - \frac{C_1 + C_2}{r} - (\frac{(\Pi_1 + \Pi_2)X_{D2}}{r - \mu} - \frac{C_1 + C_2}{r})(\frac{X}{X_{D2}})^a\Big), \tag{7}$$

where $(\frac{X}{X_{D2}})^a$ denotes the state price for default. Finally, the total firm value in this stage is the sum of D_{21}, D_{22} and E_2.

As mentioned earlier, the only decision that equityholders make in this stage is when to default. The optimal default threshold, X_{D2}, is the one that maximizes the value of equity, E_2:

$$\frac{\partial E_2(X, C_1, C_2)}{\partial X}\Big|_{X = X_{D2}} \;=\; 0, \tag{8}$$

which yields a closed-form solution for the endogenous default threshold in the second stage:

$$X_{D2} \;=\; \frac{a\,(C_1 + C_2)\,(r - \mu)}{r\,(a - 1)\,(\Pi_1 + \Pi_2)}. \tag{9}$$

[10] See e.g. Goldstein, Ju, and Leland (2001) and Hackbarth, Hennessy, and Leland (2007) for details.

[11] We use equal priority for D_{2i}. See e.g. Hackbarth and Mauer (2012) for other priority structures.

2.2.2 Adolescent Firm (Stage 1)

In the first stage, only the second investment option has not yet been exercised. The adolescent firm has assets-in-place and its capital structure consists of a mixture of debt, D_1, and equity, E_1. It has an option to default, an option to invest, and it can issue additional debt, so it solves a joint financing and investment problem. That is, when cash flows rise to the investment threshold, X_{S2}, equityholders exercise the second investment option and issues D_{22}. On the other hand, equityholders default if cash flows decline to the default threshold, X_{D1}.

The values of debt, D_1, and equity, E_1, have solutions similar to the ones in equation (1) and (3), but obey different boundary conditions. When $X \downarrow X_{D1}$, debtholders receive the liquidation value: $D_1(X_{D1}, C_1, C_2) = \frac{(1-\alpha)(1-\tau)\Pi_1 X_{D1}}{r-\mu}$. If the firm keeps growing and X rises to the investment threshold, X_{S2}, equityholders exercise the second-stage investment option, and the value of the first debt issue satisfies: $D_1(X_{S2}, C_1, C_2) = D_{21}(X_{S2}, C_1, C_2)$. For $X_{D1} \leq X \leq X_{S2}$, these value-matching conditions imply the following solution for the value of first debt issue in stage 1:

$$\begin{aligned} D_1(X, C_1, C_2) \;=\; & \frac{C_1}{r}\Big(1 - L(X) - (\frac{X_{S2}}{X_{D2}})^a H(X)\Big) + (1-\alpha)(1-\tau)\Big(\frac{\Pi_1 X_{D1}}{r-\mu} L(X) + \\ & \frac{C_1}{C_1 + C_2}\frac{(\Pi_1 + \Pi_2)X_{D2}}{r-\mu}(\frac{X_{S2}}{X_{D2}})^a H(X)\Big), \end{aligned} \tag{10}$$

where

$$L(X) \;=\; \frac{X^z X^a_{S2} - X^a X^z_{S2}}{X^z_{D1} X^a_{S2} - X^a_{D1} X^z_{S2}} \quad \text{and} \quad H(X) \;=\; \frac{X^z_{D1} X^a - X^a_{D1} X^z}{X^z_{D1} X^a_{S2} - X^a_{D1} X^z_{S2}} \tag{11}$$

denote state prices for default and investment. Intuitively, debt value, D_1, is the weighted average of the present value of the coupon payments C_1 up until default in either the first or the second stage, and the liquidation value that debtholders get when equityholders default in either stage.

Equity value E_1, on the other hand, approaches zero when $X \downarrow X_{D1}$: $E_1(X_{D1}, C_1, C_2) = 0$. As $X \uparrow X_{S2}$, it satisfies $E_1(X_{S2}, C_1, C_2) = E_2(X_{S2}, C_1, C_2) - [F_2 - D_{22}(X_{S2}, C_1, C_2)]$, because the fixed investment cost, F_2, is funded by a mixture of additional debt and equity. For $X_{D1} \leq X \leq X_{S2}$, these value-matching conditions yield the following solution for the value of equity in stage 1:

$$\begin{aligned} E_1(X, C_1, C_2) \;=\; & (1-\tau)\Big[(\frac{\Pi_1 X}{r-\mu} - \frac{C_1}{r}) - (\frac{\Pi_1 X_{D1}}{r-\mu} - \frac{C_1}{r})L(X) + \Big(\frac{\Pi_2 X_{S2}}{r-\mu} - \frac{C_2}{r} - \\ & \frac{F_2 - D_{22}(X_{S2}, C_1, C_2)}{1-\tau} - (\frac{(\Pi_1 + \Pi_2)X_{D2}}{r-\mu} - \frac{C_1 + C_2}{r})(\frac{X_{S2}}{X_{D2}})^a\Big) H(X)\Big]. \end{aligned} \tag{12}$$

The first two terms in square brackets of equation (12) denote the present value of after-tax cash flows to equityholders until equityholders default in the current stage. The next few terms in

this equation show the value from entering the next stage. Given the value of E_1, equityholders determine the optimal default threshold, X_{D1}, by maximizing equity value:

$$\frac{\partial E_1(X, C_1, C_2)}{\partial X}\Big|_{X=X_{D1}} = 0. \tag{13}$$

Similarly, the optimal investment threshold, X_{S2}, solves the smooth-pasting condition:

$$\frac{\partial E_1(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S2}} = \frac{\partial E_2(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S2}} + \frac{\partial D_{22}(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S2}}. \tag{14}$$

2.2.3 Juvenile Firm (Stage 0)

In the initial stage, the juvenile firm has no assets-in-place, an option on a two-stage investment project, and no pre-existing debt.[12] The value of equity in this stage, E_0, has a solution similar to the one in equation (3) but without the last term on the right-hand side. As $X \downarrow 0$, equity value goes to zero: $E_0(0, C_1, C_2) = 0$. When X touches the investment threshold X_{S1} for the first time from below, the option is exercised, and debt and equity finance the exercise cost, F_1: $E_0(X_{S1}, C_1, C_2) = E_1(X_{S1}, C_1, C_2) - [F_1 - D_1(X_{S1}, C_1, C_2)]$. For $X \leq X_{S1}$, this yields the following solution:

$$\begin{aligned} E_0(X, C_1, C_2) \;=\; & (1-\tau)(\frac{X}{X_{S1}})^z \Big[(\frac{\Pi_1 X_{S1}}{r-\mu} - \frac{C_1}{r}) - \frac{F_1 - D_1(X_{S1}, C_1, C_2)}{1-\tau} - \\ & (\frac{\Pi_1 X_{D1}}{r-\mu} - \frac{C_1}{r})L(X) + \Big(\frac{\Pi_2 X_{S2}}{r-\mu} - \frac{C_2}{r} - \frac{F_2 - D_{22}(X_{S2}, C_1, C_2)}{1-\tau} - \\ & (\frac{(\Pi_1+\Pi_2)X_{D2}}{r-\mu} - \frac{C_1+C_2}{r})(\frac{X_{S2}}{X_{D2}})^a\Big)H(X)\Big]. \end{aligned} \tag{15}$$

Equity value in this stage equals the present value of after-tax cash flows conditional on exercise of the first-stage option until equityholders default in stage 1 (the first three terms in square brackets of equation (15)). If cash flows grow further and the firm expands a second time, then it enters into stage 2 with the added value given by the next few terms in square brackets of equation (15).

In this stage, equityholders' choose when to invest and how much debt and equity to issue to finance the investment cost, F_1. When X is low, the benefit from exercising the option is outweighed by the value of waiting-to-invest, hence the equityholders keep the option alive. When X rises sufficiently, equityholders exercise the first option at X_{S1}, which solves the smooth-pasting condition:

$$\frac{\partial E_0(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S1}} = \frac{\partial E_1(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S1}} + \frac{\partial D_1(X, C_1, C_2)}{\partial X}\Big|_{X=X_{S1}}. \tag{16}$$

Finally, the debt coupons C_1 and C_2 maximize initial equity value, $E_0(X_0, C_1, C_2)$, subject to the above-mentioned smooth-pasting conditions for the thresholds X_{S1}, X_{S2}, X_{D1} and X_{D2}.[13]

[12] We relax this assumption in Appendix A and Section 5.3 to examine the variation in the initial debt coupon, C_0.

[13] For brevity's sake, we suppress the non-linear equations (13), (14), and (16) that determine X_{D1}, X_{S2}, and X_{S1}.

2.3 Solution of the Single-Stage Model

When $X \uparrow \infty$ in the last stage, the firm becomes risk-less, so its equity value $E_{B1}(X, C)$ and its debt value $D_{B1}(X, C)$ converge to the present value of perpetual dividend and interest payments. On the other hand, when $X \downarrow X_D$, equityholders default, and debtholders obtain the entire liquidation value (net of bankruptcy costs). In the initial stage, the firm has a single investment option, so firm value equals the value of this option. If X decreases to zero, the option becomes worthless: $E_{B0}(0, C) = 0$. But if X rises to the investment threshold, X_S, the option is exercised: $E_{B0}(X_S, C) = E_{B1}(X_S, C) - [F - D_{B1}(X_S, C)]$.

The above-mentioned boundary conditions yield the following solutions for $X \geq X_D$:

$$D_{B1}(X, C) = \frac{C}{r}\Big[1 - (\frac{X}{X_D})^a\Big] + (1-\alpha)(1-\tau)\frac{\Pi X_D}{r-\mu}(\frac{X}{X_D})^a, \tag{17}$$

$$E_{B1}(X, C) = (1-\tau)\Big[\frac{\Pi X}{r-\mu} - \frac{C}{r} - (\frac{\Pi X_D}{r-\mu} - \frac{C}{r})(\frac{X}{X_D})^a\Big], \tag{18}$$

and for $X \leq X_S$:

$$E_{B0}(X, C) = \Big[(1-\tau)\frac{\Pi X_S}{r-\mu} + \frac{\tau C}{r} - F - [(1-\tau)\frac{\Pi \alpha X_D}{r-\mu} + \frac{\tau C}{r}](\frac{X_S}{X_D})^a\Big](\frac{X}{X_S})^z. \tag{19}$$

The optimal default threshold, X_D, maximizes the value of equity, E_{B1}, that is:

$$\frac{\partial E_{B1}(X, C)}{\partial X}\Big|_{X=X_D} = 0, \tag{20}$$

which implies the following closed-form solution:

$$X_D = \frac{a\,C\,(r-\mu)}{(a-1)\,\Pi\,r}. \tag{21}$$

The optimal investment threshold, X_S, also maximizes the value of equity, E_{B1}, that is:

$$\frac{\partial E_{B0}(X, C)}{\partial X}\Big|_{X=X_S} = \frac{\partial E_{B1}(X, C)}{\partial X}\Big|_{X=X_S} + \frac{\partial D_{B1}(X, C)}{\partial X}\Big|_{X=X_S}. \tag{22}$$

Finally, debt coupon C maximizes in initial equity value, E_{B0}, subject to the above-mentioned smooth-pasting conditions for the thresholds X_D and X_S.

3 Financial Flexibility and the Investment Process

This section studies the key difference between the multi-stage model and the single-stage model (i.e. the intermediate stage of an adolescent firm). This intermediate stage links financial flexibility to the structure of the investment process. We illustrate how financing and investment decisions of the adolescent firm influence those of the mature firm and vice versa.

3.1 Intertemporal Effect

In the multi-stage model, suppose equityholders issue more debt in the first stage (i.e. C_1 is higher). This means that equityholders will bear less of the investment cost (i.e. $F_1 - D_1$ is lower). This reduction in the equity-financing of the exercise cost expedites the exercise of the first option. As a result, the firm produces first-stage cash flows, in expectation, earlier, which translates into a higher initial equity value, E_0. A higher C_1, however, reduces financial flexibility going forward. Therefore, the firm has to wait longer to exercise the second option and to receive second-stage cash flows, which translates into a lower initial equity value, E_0. Thus, the level of C_1 has two opposing forces in the multi-stage model, and the optimal level strikes a balance between the two forces.

On the other hand, suppose equityholders issue more debt in the second stage (i.e. C_2 is higher). This means that the firm uses more debt to fund the second-stage investment cost and hence equityholders bear less of the investment cost (i.e. $F_2 - D_{22}$ is lower). This expedites the exercise of the second option, raises the expected present value of cash flows from the second stage, and increases initial equity value, E_0. But the firm is more likely to go bankrupt when there is more second-stage debt, which decreases the expected present value of cash flows from the second stage. In addition, the anticipation of the higher second-stage debt level lowers financial flexibility in the first stage. This delays the exericise of the first-stage option and decreases initial equity value, E_0. So, the optimal level of C_2 also trades off two opposing forces on initial equity value that follow from the dynamic interactions between financing and investment decisions in the multi-stage model.

Dynamic financing-investment interactions between the adolescent and mature stages lead to an "intertemporal effect," i.e. reaping exercise (i.e. cash flow) benefits from issuing debt in stage 1 against retaining financial flexibility for funding more of the investment cost with debt in stage 2.[14] To illustrate the intertemporal effect, we select economically plausible base case parameter values. The initial cash flow level, X_0, is set to \$5 and the risk-free rate equals $r = 6\%$. The growth rate of X is $\mu = 1\%$ and the volatility of X is $\sigma = 25\%$, which are close to estimates by Morellec et al. (2012). The bankruptcy cost is $\alpha = 30\%$ and the effective corporate tax rate is $\tau = 10\%$.[15] The scales of the investment options are $\Pi_1 = 1$ and $\Pi_2 = 1$, and the investment costs are $F_1 = \$100$ and $F_2 = \$200$.

[14] This does not depend on bankruptcy costs or taxes, which are constant over time and hence cannot cause timing differences. As we will see, the intertemporal effect is largely attributable to the structure of the investment process.

[15] This tax rate is lower than those used in other studies. We do this on purpose, because we want to limit tax effects and emphasize the intertemporal effect due to the structure of the investment process. In addition, structural estimation of the multi-stage model in Section 4 provides fairly low point estimates of the effective corporate tax rate.

Using this base case environment, Figure 1 displays the intertemporal effect by mapping debt coupon pairs, C_1 and C_2, into initial equity value, E_0, on the basis of equation (15). The figure reveals that E_0 is convex C_1 and C_2 and, in particular, that an *interior optimum* is clearly present. Thus, the intuition behind the intertemporal effect discussed above leads indeed to an optimal pair of (C_1, C_2) that corresponds to the highest attainable point of initial equity value on the surface.

[Insert Figure 1 Here.]

Table 2 reports, for the base case environment, optimal capital structure choices, investment thresholds, default thresholds, and market leverage ratios. Market leverage is defined as the ratio of market value of debt over the sum of market value of debt and market value of equity. Panel A tabulates the optimization results for the single-stage model, while Panel B shows the corresponding outputs for the multi-stage model. One of the key differences between the first column in Panel B and the first two columns in Panel A is the role played by financial flexibility.[16] That is, the underutilization of debt capacity, which we can gauge by the difference in leverage ratios between the single-stage model (42%) and the multi-stage model (28% and 38%), shows that the firm in the multi-stage model has a strong incentive to retain financial flexibility in the first stage. In addition, the firm in the multi-stage model continues to have a lower target leverage ratio in the second stage. That is, underutilization persists and leverage ratios are lower in both stages of the multi-stage model relative to the ones of an otherwise identical firm in the single-stage model.

[Insert Table 2 Here.]

It is remarkable that leverage does not vary with nature of the investment option in the single-stage model (Panel A). Hence the underutilization of debt in the multi-stage model (Panel B) is closely related to the intertemporal effect. On the one hand, using more debt to finance the first investment lowers equityholders' contribution to the first investment cost, so equityholders will invest earlier (i.e. at a lower investment threshold). On the other hand, the pre-existing debt issued in the first stage creates default risk and reduces financial flexibility in the second stage, so equityholders will invest later (i.e. at a higher investment threshold). These countervailing forces lead to a variety of realistic outcomes, which depend crucially on the relative size of the investment scales, Π_1 and Π_2. In particular, the results in Table 2 indicate that equityholders underutilize debt in stage 1 to maximize the value of their financing and investing options. Absent any other frictions

[16] Note that in Panel A the benchmark model's investment cost, F, equals either \$100 or \$200 to make it comparable to the first or the second stage of multi-stage model in Panel B. The same applies to the choice of investment scales.

(e.g. agency conflicts or transaction costs), optimization generates path-dependent and persistent leverage ratios in a dynamic trade-off model that incorporates irreversible investment.

In sum, these findings imply that structural models without dynamic financing-investment interactions (1) overestimate target leverage ratios, and (2) can be misleading in that they imply a fixed target leverage ratio that is largely taken to be exogenous to the investment process. The latter point also suggests that there is no meaningful measurement of partial adjustment towards target leverage without recognition of firm-level heterogeneity in the investment process. Therefore, we examine the role of the structure of the investment process in the next subsection.

3.2 Structure of the Investment Process

To study how leverage changes with the structure of the investment process, we modify the base case of $\Pi_1 = 1$ and $\Pi_2 = 1$ (see first column in Panel B of Table 2) in columns 2–4. Column 2 depicts optimization results for a back-loaded investment structure ($\Pi_1 = 0.75$ and $\Pi_2 = 1.25$), while column 3 contains a front-loaded one ($\Pi_1 = 1.25$ and $\Pi_2 = 0.75$). Finally, column 4 reports the corresponding outcomes for a very front-loaded investment structure ($\Pi_1 = 1.5$ and $\Pi_2 = 0.5$).[17]

These columns highlight several interesting features of the multi-stage model. First, the firm retains less (more) financial flexibility in the first stage when the structure of the investment process is front-loaded (back-loaded). For example, if we reduce the first-stage investment scale by 25% and raise the second-stage investment scale by 25%, then leverage in stage 1 decreases substantially from 28% to 20% (a decline of almost a third) and leverage in stage 2 increases from 38% to 40%. This result for the first stage helps explain the debt conservatism puzzle (see Graham (2000)).

Second, the difference in target leverage ratios across the two stages declines (rises) when the structure of the investment process is front-loaded (back-loaded). Consider the case in column 2, where 25% of the first-stage investment scale are pushed into the second stage, so the structure of the firm's investment process is more back-loaded than in the base case of column 1. As a result, the difference in target leverage ratios effectively doubles (it increases from 10% to 20%). Hence firms that only differ in terms of their investment options (i.e. are otherwise identical) neither have the same target leverage nor follow the same leverage dynamics in the multi-stage model.

Third, the results in Panel B indicate that typically first-stage leverage is lower than second-

[17] Changing Π_1 and Π_2 in lock step produces the same coupons and leverage ratios as in column 1. All else equal, only the *ratio* of Π_1 and Π_2 matters because of of the scaling property. So we only consider asymmetric changes.

stage leverage, which is consistent with dynamic capital structure models without investment (see e.g. Goldstein, Ju, and Leland (2001) and Strebulaev (2007)). However, a sufficiently front-loaded investment process produces higher leverage in stage 1 than in stage 2 (see column 4). Intuitively, there is very little incentive to retain financial flexibility in this case and hence the firm utilizes its debt capacity more aggressively already in the first stage. Thus, unlike dynamic capital structure models without investment, the multi-stage model can produce increasing and decreasing leverage ratios over time, which are largely driven by the structure of the firm's investment process.

Finally and related to the previous point, it is perhaps also surprising that the mature firm with front-loaded investments selects lower leverage in the second stage (see columns 3 and 4) relative to the base case (see column 1). As in Childs et al. (2005), lower leverage ratios in later stages could be due to increases in the firm's asset risk (e.g. because mature markets tend to be more competitive and hence riskier). It turns out, however, that even when the firm's asset risk is constant over time leverage ratios can nevertheless decline over time.

Overall, the analysis shows how incentives to retain financial flexibility in the first stage crucially depend on the investment process. The lower the first-stage investment scale, Π_1, is relative to Π_2, the more the firm saves debt capacity in stage 1. Given the wide range of optimal (target) leverage ratios, the results in Table 2 suggest that leverage ratios can greatly vary depending on how the firm grows assets-in-place by exercising its real options. Therefore, it is difficult to determine target leverage in the conventional sense unless the structure of investment process is recognized in future empirical studies on target leverage and speed of adjustment to target leverage. In addition, financing-investment dynamics in the multi-stage model produce a significant fraction of low (and zero) leverage firms and also path-dependent, persistent leverage ratios (see also Section 5.3).

3.3 Other Comparative Statistics

We implement a sensitivity analysis on how dynamic financing-investment interactions and leverage ratios change with parameter values unrelated to the investment process. We vary the effective corporate tax rate, τ, the bankruptcy cost, α, the cash flow volatility, σ, and the cash flow growth rate, μ. In particular, we increase and decrease each parameter by 50% of its base case value, while keeping the other parameters unchanged. Similar to Table 2, Table 3 reports optimal debt coupons, investment thresholds, default thresholds, and market leverage ratios.

[Insert Table 3 Here.]

Not surprisingly, leverage goes up in both stages if the effective corporate tax rate, τ, rises. This follows from trade-off theory, because higher taxes lead to higher tax benefit of debt. The firm issues more debt and hence defaults earlier. The net effect of more debt issuance and more default risk is that optimal investment thresholds do not respond much to higher tax rates. The bankruptcy cost, α, has a negative impact on the value of debt, so it works in the opposite direction. Because higher bankruptcy costs lower the firm's debt capacity to fund the investment expenditure, investment takes place, in expectation, later. Yet, similar to the role of taxes, bankruptcy costs are also more related to debt and hence investment thresholds do not change significantly. Finally, notice that leverage ratios are sensitive to both changes in bankruptcy costs and changes in tax rates.

Since the volatility of cash flows, σ, is a measure of uncertainty, the investment option's value rises with σ and, as a result, optimal investment occurs, in expectation, later. In the multi-stage model, initial equity value equals the value of a sequential investment (compound) option. Therefore, changes in volatility greatly change investment decisions. When volatility goes up, it is more valuable to keep the option alive, so the firm waits longer to invest in both stages (X_{S1} rises from 12.36 to 17.51 in stage 1 and X_{S2} rises from 23.67 to 33.08 in stage 2 for the case in column 6). Consistent with many studies building on Leland (1994), varying volatility also leads to significant variation in leverage. When volatility is high, the firm is riskier (i.e. more likely to go bankrupt) and hence uses debt more conservatively in both stages and leverage ratios drop significantly relative to the base case. Thus, it can pose a challenge for structural estimation that volatility strongly affects both financing and investment decisions.

Finally, a higher growth rate of cash flows, μ, also makes the firm's options more valuable, because their intrinsic value is higher for any level of cash flows and hence waiting to invest becomes costlier. A rise in μ leads to, in expectation, earlier investment (i.e. X_{S1} declines from 12.36 to 11.99 in stage 1 and X_{S2} declines from 23.67 to 22.91 in stage 2 as seen in column 8). A rise in μ also leads more debt-financed investment in both stages. However, leverage ratios are fairly insensitive to changes in the growth rate, which might also make structural estimation of μ more challenging.

For the base parameter values, the multi-stage model produces leverage ratios, which closely match those observed in practice. In the next section, we tackle the question whether several simulated model moments can simultaneously match a number of desirable data moments for a set of estimated parameter values. While the sensitivity analysis in this section sheds additional light on model, it also helps us find informative moments for estimating parameters in the next section.

4 Simulated Moments Parameter Estimation

To test the model's ability to match observed outcomes, we turn to simulation methods based on indirect inference techniques in Gourieroux, Monfort, and Renault (1993) and Gourieroux and Monfort (1996). Like Hennessy and Whited (2005, 2007), we use Simulated Method of Moments (SMM) to estimate a set of structural parameters of the model. To do so, we solve the multi-stage model numerically and then use this solution to generate simulated panels of firms. SMM selects parameter values by minimizing the distance between moments from actual data and corresponding moments from simulated data. That is, the goal of SMM is to find an optimal vector of unknown structural parameters, say b^*, by matching a set of simulated *model moments* with corresponding *data moments*.

Let $b = (\Pi_1, \Pi_2, \alpha, \tau)$ be the vector of unknown structural parameters to be estimated by SMM. We simulate $S = 6$ artificial panels data sets consisting of $N = 1,000$ firms for 200 years using the multi-stage model and a given b. In each panel, we only keep $T = 100$ years (or 400 quarters given that $\Delta t = 0.25$) after discarding the first 100 years to avoid undue influence of initial conditions. Once a firm defaults, we replace it by a new firm with the same characteristics to keep the size of the simulated data sets constant over time. By iterating b and calculating the distance between the model moments, M_m, and data moments, M_d, we estimate the optimal vector of parameters, b^*.[18]

The moments to match are selected such that they are *a priori* informative about the unknown structural parameters, b. Intuitively, a moment is informative about b if it can identify at least some elements in b, which means it is sensitive to changes in b. Informative moments enable SMM to converge faster and to provide more robust economic insights. We select the following five moments to estimate the four structural parameters $(\Pi_1, \Pi_2, \alpha, \tau)$:[19]

1. Quasi-Market Leverage (QML): Let QML_t^i denote the quasi-market leverage ratio (i.e. the book value of debt divided by the sum of market value of equity and book value of debt) of the simulated firm i, with $i = 1...N$, at time t, with $t = 1..., T$. We first calculate the cross-sectional average for every time t and then take the average of the cross-sectional averages over time, i.e. $QML = \frac{1}{T}\sum_{t=1}^{T}(\frac{1}{N}\sum_{i=1}^{N} QML_t^i)$. This moment reflects how the net benefits of debt and, in particular, the structure of the investment process affects the level leverage. So we expect it to be sensitive to e.g. Π_1 and also responsive to α and τ.
2. Dispersion of Quasi-Market Leverage ($DispQML$): This moment is defined as the cross-

[18] See Strebulaev and Whited (2012) for benefits and relevance of indirect inference techniques in corporate finance.
[19] Appendix B provides a more detailed description of the structural estimation procedure that we implement here.

sectional average of the time-series standard deviations of firms' quasi-market leverage ratios, i.e. $DispQML = \frac{1}{N}\sum_{i=1}^{N}\sqrt{\mathrm{Var}_i(QML_1^i, ..., QML_T^i)}$. This moment reflects how firms respond to shocks when optimally financing their investment projects. Hence this moment is also likely to be informative about Π_1 as well as α and τ, but it captures cross-firm variation in leverage.

3. Debt Issuance (D/K): We compute D/K as the ratio of net debt issuance to capital at investment points. This moment reflects the proportion of debt used to finance investment expenditures, which is higher if bankruptcy costs are lower or if tax rates are higher. It should be sensitive to the parameters α and τ that determine the net benefits of debt issuance.
4. Market-to-Book (Q): We first calculate the cross-sectional average for every time t and then take the average of the cross-sectional averages over time, i.e. $Q = \frac{1}{T}\sum_{t=1}^{T}(\frac{1}{N}\sum_{i=1}^{N} Q_t^i)$, where Q_t^i is the market value of firm i divided by the book value of firm i at time t. Q proxies for investment opportunities and hence it should be informative about Π_1 and especially Π_2.
5. Investment-to-Equity (Inv/Eq): This moment is defined as investment cost (i.e. F_1 or F_2) divided by book value of equity at investment points. Since the investment costs are fixed, this moment depends more on when the firm exercises its options and, in particular, how high equity value has to rise for exercise to be optimal. Therefore, it is likely related to Π_1 and Π_2, but potentially also to τ because equity is a claim on after-tax cash flows.

Table 4 presents the sensitivities of the five moments to changes in the model parameters b. The base case scenario is in the first column. In the other columns, each of the four parameters, namely Π_1, Π_2, α and τ, is separately increased by 50%. Panel A displays the absolute changes of the moments and Panel B shows percentage changes relative to the base case in the first column. The table reveals that QML and $DispQML$ are indeed most sensitive to Π_1. This is because QML reflects the investment and financing activities in the past, i.e. the level and dispersion of early stage leverage ratios are primarily determined by how high Π_1 is. Tax rate τ and bankruptcy cost α most strongly affect the debt issuance moment, D/K, because they are the key determinants of both debt capacity and net tax benefits. Q is very sensitive with respect to changes in Π_2. Recall that initial equity value corresponds to a compound option in the multi-stage model. All else equal, firms with more a back-loaded investment process (i.e. higher Π_2) will have much higher market-to-book ratios. The investment to book equity ratio Inv/Eq responds the most to τ and Π_2 and also a bit less so to Π_1. In sum, Π_1 influences mainly QML and $DispQML$, Π_2 matters the most for Q and also changes D/K, α and τ have the strongest effect on D/K but also affect

QML, and finally τ (but not α) impacts Inv/Eq.

[Insert Table 4 Here.]

We use the COMPUSTAT annual tape for the 45-year period between 1965 and 2009 to estimate the data moments.[20] We refer to this vector as the "Full Sample" moments. We run SMM also on various subsamples to provide insights into the structure of companies' investment process. Therefore, the COMPUSTAT sample is split into three subsamples according to Q. For each firm-year, firms are ranked by the value of Q from the lowest to the highest. Firms in the lowest 33% of the distribution are classified as the "Low Q" sample, firms in the highest 33% belong to the "High Q" sample, and those in between are in the "Medium Q" sample. For each of the subsamples, we also compute the corresponding data moments. We then run SMM for each of the four samples and collect the vector of structural parameter estimates, b^*, along with the (fitted) model moments.

The parameter estimates for the full sample and the three subsamples are presented in Panel A of Table 5. The numbers in the parentheses are the standard deviations of model estimates across the 1,000 panels with the exception of the χ^2 test, for which that number is the p-value for the overidentification test. In particular, the χ^2 test of the overidentifying restrictions does not produce a rejection at the 10% level for any of the four structural estimations in Panel A. Panel B of Table 5 reports the data moments and the fitted (model) moments for the full sample and the three subsamples. For all four estimations, the fitted moments are very close to the data moments. This implies that the simulated economy with these parameter estimates closely mimics the real economy.

[Insert Table 5 Here.]

As argued earlier, the ratio of investment scales, Π_2/Π_1, captures the structure of investment process. Panel A reveals that the "High Q" sample has a fairly back-loaded investment processes ($\Pi_2/\Pi_1 = 2.284 > 1$), whereas the other three samples display various front-loaded investment processes. For example, the "Low Q" sample shows the most front-loaded investment process ($\Pi_2/\Pi_1 = 0.175 < 1$), which is also the only case of Π_1 not being reliably measured. Importantly, these results of the structural estimation are consistent with the theoretical discussion in Section 3.2.

Specifically, firms in the "High Q" sample tend to have many future investment opportunities and thus large growth potential — the structure of the investment process of these firms is indeed

[20] We remove financial firms (SIC between 6000 and 6999) and utilities (SIC between 4900 and 4999), because they operate in regulated industries. We also remove firm-year observations with total assets less than two million and plant, property, and equipment less than one million to avoid biases caused by small firms.

back-loaded, so they initially retain more financial flexibility (i.e. save more debt capacity). This is why we observe the lowest leverage ratio for this sample. The "Low Q" sample has more mature firms and they do not have many future investment opportunities. Their investment process tends to be more front-loaded, so they do not have a motive to save debt capacity for future investments and this is why we observe the highest leverage ratio for this sample. On average, the 45-year COMPUSTAT sample contains more firms having fairly front-loaded investment process.

Another interesting observation is that the estimated tax rate, τ, is low for all four samples, ranging from 4% to 7%. There is more variation in the estimates of the bankruptcy costs, α, but if we put less weight on the "Low Q" sample, then it is also roughly 30%. This implies that the net tax benefit of debt is not driving the result, confirming the conclusion of Section 3. While, these findings are also consistent with the debt conservatism puzzle in that the data moments of observed leverage ratios are in line with relatively low effective tax rates, they establish, more importantly, that the structure of the investment process is likely to be a more important determinant of leverage ratios than tax rates or bankruptcy costs, because the SMM indicates that its parameters, Π_1 and Π_2, vary much more widely across subsamples than α and τ.

To summarize, unobserved heterogeneity in terms of the precise structure of the investment process (e.g. front-load, mid-loaded, or back-loaded) seems to be large and important for understanding the cross-sectional distribution of corporate investment and financing decisions within an industry or for the entire economy. Thus, future capital structure research should try to move more into the direction of recognizing and treating this important source of cross-firm heterogeneity.

5 Capital Structure Tests

Simulation is a useful tool for testing theoretical models (see e.g. Hennessy and Whited (2005), Leary and Roberts (2005), Strebulaev (2007), and Tserlukevich (2008)). In this section, we investigate the cross-sectional properties of leverage ratios in dynamic, simulated economies where firms make endogenous investment and financing decisions. We compare capital structure regression results for simulated data to the corresponding results for real data. Finally, we perform leverage portfolio sorts used for COMPUSTAT data by Lemmon, Roberts, and Zender (2008) for simulated data.

5.1 Panel Simulations

We begin by detailing the procedure of simulating dynamic economies with heterogeneous firms. The simulations take solutions for the valuation equations and, in particular, for the optimal investment and financing decisions in Section 2.2 as given and do not involve any additional optimizations.

It is well-known that systematic (or economy-wide) and idiosyncratic (firm-specific) shocks have explanatory power for leverage ratios. The former create cross-firm dependencies in dynamic economies. Hence we decompose the cash flow process into systematic and idiosyncratic components to allow for a more realistic correlation structure:

$$dX_i(t)/X_i(t) \;=\; \mu\, dt + \beta_i\, \sigma_S\, dW^S(t) + \sigma_{Ii}\, dW_i^I(t),\;\; X_i(0) = X_0 > 0,\;\; i = 1, ..., N,\;\; t = 1, ..., T \quad (23)$$

where constants σ_S and σ_{Ii} represent, respectively, volatilities of systematic and idiosyncratic shocks. The stochastic processes $dW^S(t)$ and $dW_i^I(t)$ are independent Wiener processes, $dW(t) = \beta_i\, dW^S(t) + dW_i^I(t)$, and the parameter β_i measures firm i's exposure to systematic shocks. Thus, the total risk can be calculated as $\sigma_i = (\sigma_{Ii}^2 + \beta_i^2 \sigma_S^2)^{\frac{1}{2}}$.

Based on a discretization of equation (23), we simulate 1,000 panel data sets with $N = 3,000$ firms for $T = 400$ quarters. More specifically, we generate 200 years of data (or 800 quarters given that $\Delta t = 0.25$) based on the multi-stage model and then drop the first 400 quarters to obtain a stationary sample for each simulated economy and to limit the influence of initial conditions. All firms in the same panel are governed by the same series of systematic shocks, $dW^S(t)$, but the dynamics of economies are different across the 1,000 panels. At time $t = 0$ of each panel, the optimal policies are determined as a function of firm characteristics (i.e. parameter values). For all $t > 0$, firms follow their optimal investment, debt and equity issuance, and default policies given that they observe the evolution of their cash flow process every quarter. If a firm defaults, it is "reborn," i.e. it is replaced in the next quarter by a juvenile firm with identical initial conditions.

Panel A of Table 6 provides an overview of the values and distributions of model parameters that are set once and for all at time $t = 0$ to produce the simulated economies. To begin, we use the structural estimation results for the full sample in Section 4. That is, the investment scales are estimated for all firms to $\Pi_1 = 1.966$ and $\Pi_2 = 1.286$. The bankruptcy cost, α, and the tax rate, τ, are uniformly distributed with means corresponding to the SMM's full sample results and ranges of +/–20% around the means. Similarly, the investment costs, F_1, and F_2, have uniform distributions with supports $[80, 120]$ and $[160, 240]$, respectively. The systematic shock is fixed to $\sigma_S = 0.148$

based on estimates reported by Schaefer and Strebulaev (2008). The idiosyncratic shock, σ_{Ii}, varies around a mean of 0.217 based on a chi-squared distribution: $\sigma_{Ii} \sim 0.05 + \frac{1}{30}\chi^2(5)$. Firm i's exposure to systematic shocks, β_i, follows a uniform distribution, whose first two moments correspond to the empirical distribution with mean of 0.993 and standard deviation of 0.47 reported by Strebulaev (2007). Finally, the other parameters assume the base case values, i.e. risk-free rate $r = 6\%$, growth rate of cash flows $\mu = 1\%$, and initial cash flow level $X_0 = \$5$.

[Insert Table 6 Here.]

Panel B of Table 6 presents the cross-sectional distribution of leverage both at investment points and across all panels (i.e. in dynamics). For each simulated data set, we first calculate statistics for each quarter. We then average across quarter within each simulated economy, and then average across economies. However, the rows "Min." and "Max." report, respectively, the minimum and the maximum assumed by the corresponding quantities. Investment points are further classified as first and second investment points, because the multi-stage model features two investment options. Market leverage, ML, is defined in Section 3.1. Quasi-market leverage, QML, equals book value of debt divided by the sum of market value of equity and book value of debt in this model, where book value of debt is defined as the value of debt at the beginning of a stage (i.e. at $X = X_{S1}$ or $X = X_{S2}$). Hence quasi-market leverage and market leverage coincide at investment points.

The table confirms that ML and QML are not very different. Across all panels, average ML is 19.7% and the average QML is only 0.8% higher. Yet, market leverage ratios at first investment points are almost half of those at second investment points, which is attributable to the strong incentive of adolescent firms to retain financial flexibility. Taken together, average leverage at investment points equals 18.7%. This is significantly lower than in similar models without endogenous investment by Goldstein, Ju, and Leland (2001) and Strebulaev (2007), who report 37% and 26%. Hackbarth and Mauer (2012) obtain optimal leverage ratios as low as 12%, but their success is largely due to debt overhang and debt (dilution) dynamics, whereas our simulations do no rely at all on agency problems. Moreover, the standard deviations of leverage ratios at investment points are about half of those for all data points. This is due to the fact that firms tend to make infrequent investments that occur at optimal times. Thus, even though target leverage ratios differ across firms, they are less dispersed than leverage ratios in dynamics. In addition, the distribution of leverage ratios at investment points are almost symmetric, whereas the ones in dynamics are right-skewed (i.e. the mean exceeds the median). Intuitively, because firms in various (investment) stages of the

model or, more generally, their life-cycle, respond differently to economic shocks of the same magnitude, the behavior of leverage ratios at investment points is quite different from that in dynamics.

In sum, the simulations of heterogeneous firms generate much lower average leverage ratios than prior work, both at the investment points and in dynamics, and yet it is still able to generate leverage ratios spanning over the $[0, 1]$ interval. Therefore, we conclude that the structure of firms' investment process is crucial for obtaining realistic distributions of leverage ratios in simulated economies. Intuitively, firms endogenously preserve debt capacity (i.e. retain financial flexibility) for future investment stages. That is, the intertemporal effect of the multi-stage model of corporate investment and financing dynamics captures an important mechanism which helps explain the low-leverage puzzle of Graham (2000). More recently, Strebulaev and Yang (2012) document a closely related, so-called zero-leverage puzzle given that e.g. 14.0% of large, public companies had no debt outstanding in the year 2000. Consistent with their findings, our model produces, on average, also produces a large and persistent fraction of zero-leverage firms. As seen from the 10th percentile in Panel B of Table 6, the fraction of zero-leverage firms in dynamics exceeds, on average, 10% for the 1,000 simulated panel data sets. Clearly, this suggest that, at the very least, the model is able to explain a substantial part, if not most, of the low- and zero-leverage puzzles. It seems that this success cannot be achieved by alternative models without endogenous investment, so considering dynamic interactions between corporate investment and financing is crucial.

5.2 Cross-Sectional Regressions

In this section, we focus on the behavior of quasi-market leverage, market-to-book, and profitability in simulated data sets. In particular, we estimate capital structure regressions both at investment points and for all observations in the panels (i.e. in dynamics). This also allows us to examine the role of other determinants of capital structure that are typically used in the empirical literature.

Growth options might have a negative debt capacity, because debt overhang rises with leverage (Myers (1977)). Indeed, numerous empirical studies find a negative relation between leverage and market-to-book, a commonly used proxy for growth options, and interpret it as evidence for agency problems. For example, Smith and Watts (1992) document a negative relation between quasi-market leverage ratios and market-to-book ratios. Similarly, Rajan and Zingales (1995) report a reliably negative relation between quasi-market leverage and the market-to-book ratio across seven different countries. However, they conclude: "From a theoretical standpoint, this evidence

is puzzling. If the market-to-book ratio proxies for the underinvestment costs associated with high leverage, then firms with high market-to-book ratios should have low debt..." Yet, Chen and Zhao (2006) find leverage is positively related to market-to-book for all firms except those with the highest market-to-book ratios. We therefore study the leverage-growth relation in our simulated economies.

A distinct yet related line of research studies the relation between leverage and profitability. Myers (1993) argues that the negative relation between leverage and profitability is one of the most pervasive patterns of empirical capital structure research. According to Strebulaev (2007), it is also one of a few relations that enables us to distinguish between the (static and dynamic) trade-off model and pecking order behavior. We therefore examine whether conclusions from prior research on the leverage-profitability relation in dynamic capital structure models without investment carry over to the simulated data sets, in which corporate investment and financing are endogenous.

More specifically, the empirical variables of interest are profitability, π, and market-to-book, Q. The interaction of leverage with these two factors is widely used to differentiate implications of the trade-off theory of capital structure from the pecking order. Based on the standard trade-off theory, higher profitability enables firms to reduce the costs of bankruptcy and increase the tax benefit of debt. Thus, a positive leverage-profitability relation is predicted. This prediction is challenged by a large body of empirical research, such as Titman and Wessels (1988), Rajan and Zingales (1995), and Fama and French (2002), and Baker and Wurgler (2002), who all find a negative association confirming the pecking order's prediction. Firm behavior according to the pecking order means that higher profitability allows firms to use more retained earnings. Holding investment fixed, leverage is thus lower for more profitable firms. As a result, the negative leverage-profitability relation has traditionally been regarded as evidence in favor of pecking-order and against trade-off behavior. Regarding the leverage-growth relation, these two theories have opposite predictions too. In the trade-off world, high growth firms tend to have lower collateral values and hence higher bankruptcy costs. Trade-off firms with high growth should therefore issue less debt. In the pecking-order world, debt increases when capital expenditures are higher than retained earnings, and decreases when capital expenditures are lower than retained earnings. Holding profitability fixed, leverage is thus higher for pecking-order firms with high growth. Taken together, a positive (negative) leverage-Q (or leverage-π) relation follows from pecking order (trade-off) arguments.

Recall that we generate 1,000 panel data sets with 800 quarters based on the multi-stage model and then drop the first 400 quarters to obtain a stationary sample for each simulated economy

and to limit the influence of initial conditions. Using these simulated economies, we estimate four versions of a standard capital structure regression model for quasi-market leverage:

$$QML_i = \beta_0 + \beta_1\, x_i + \beta_2\, \sigma_i + \beta_3\, \alpha_i + \beta_4\, \tau_i + \epsilon_i, \tag{24}$$

where x is either profitability, π, in Panel A of Table 7 or market-to-book, Q, in Panel B of Table 7. In Panel C of Table 7, we include both profitability, π, and market-to-book, Q, as regressors. We measure profitability, π, as earnings before interest and tax (or cash flows) scaled by firm value, whereas the market-to-book ratio, Q, is the ratio of total market value of asset over book value of asset. The other independent variables are time-invariant firm attributes: volatility of cash flows, σ, bankruptcy cost, α, tax rate, τ, and firm size, φ, which equals the sum of book value of debt and book value of equity. We focus on QML as regressand, because distributions of market leverage and quasi-market leverage closely mimic each other in the simulated economies (see Table 6).

[Insert Table 7 Here.]

In Table 7, the first column reports the regression results at investment points and the other columns report the ones on simulated economies.[21] In particular, the first version of equation (24) is the "Investment Points" regression, whose estimation results are tabulated in the first column (Inv. Pts.) of Table 7.[22] The second column (BJK) of Table 7 reports OLS regression results in the fashion of Bradley, Jarrel, and Kim (1984). The dependent variable, QML_i, is calculated as the sum of book values of debt over the 400 quarters divided by the sum of book values of debt and market values of equity over the 400 quarters. The independent variables are calculated similarly (if possible). Note that for this regression the dependent variable and independent variables are contemporaneous. In the third column (RZ), the independent variables are averaged over quarters $t-1$ to $t-4$ to reduce noise as in Rajan and Zingales (1995), while the dependent variable, QML_i, is measured at time t. Finally, the fourth column (FF) adopts the Fama-MacBeth regression approach as in Fama and French (2002). At each time t, QML is regressed on lagged independent variables. We report averages of the quarter-by-quarter coefficient estimates along with Fama-MacBeth standard errors that are corrected with the Newey-West method.

Strebulaev (2007) points out empirical capital structure regressions should differentiate refinancing points from other data points. He develops a dynamic trade-off model with financing frictions,

[21] Coefficient estimates and t-statistics reported in this table are the averages across the 1,000 simulated economies.

[22] In Strebulaev (2007), the first regression is run at refinancing points only as he considers only financing friction. Our paper considers only investment frictions. In reality, one would, however, expect both frictions to be important.

where firms size if fixed over time. An important question is therefore whether similar conclusions obtain if firm size is not fixed over time, so firms can make a sequence of endogenous investment and financing decisions. To this end, Table 7's Panel A reveals that the leverage-profitability relation is positive and significant at investment points (see first column), which is consistent with static trade-off behavior. Interestingly, it is reliably negative in the other columns, in which we estimate BJK, RZ, and FF regressions using all data points (i.e. in dynamics). This is the pecking order's prediction, but derives entirely from data produced by a dynamic trade-off model with investment frictions. The effects of cash flow volatility, bankruptcy cost, tax rate, and firm size on leverage are also significant and go in the expected directions. The upshot of Panel A is that infrequent, lumpy investment provides an economically important alternative to financing frictions, because we observe remarkably different patterns at investment points versus in dynamics.

Furthermore, the intertemporal effect of the multi-stage model has implications for the leverage-growth relation, which we examine in Panel B of Table 7. For example, Frank and Goyal (2009) summarize that market-to-book has a reliably negative relation with leverage, which is consistent with the prediction of both trade-off theory and market-timing theory. Absent agency problems or market inefficiencies, this phenomenon is strongly borne out in the regressions on all data points (i.e. in dynamics). Again, the sign is reversed at investment points. Thus, the interpretation of cross-sectional tests of the leverage-Q relation changes depending on whether firms are active (i.e. at investment points) or passive (i.e. in between investment points). While firm size, φ, and firm risk, σ, are both economically and statistically significant in Panel B, bankruptcy cost, α, and tax rate τ are less reliable variables, consistent with Frank and Goyal (2009). Consider, for example, the RZ regressions, where α and τ are not even 10% significant. In contrast, α and τ are highly significant in Strebulaev (2007), where Q is not included as independent variable in the regression analysis.

Finally, Panel C includes both profitability, π, and market-to-book, Q, as regressors. The results are similar to the ones in Panels A and B. Interestingly, neither π nor Q lose statistical power, even though both are influenced by the same underlying sources of uncertainty. Thus, this last part of the regression analysis suggests that profitability and market-to-book are independently important for explaining the behavior of leverage ratios. More generally, we expect in reality both financing frictions and investment frictions. So, these complementary types frictions will be present at different points in time (i.e. at separate investment and refinancing points) and also at the same points in time as assumed by the model. Clearly, this can only strengthen the relevance of our conclusions.

To summarize, the regression results based on simulated data using our structural estimation results are able to replicate stylized facts established by empirical research. In the spirit of Strebulaev (2007), simulation of the multi-stage model of corporate investment and financing dynamics reinforces the need to differentiate investment points from other data points when studying corporate behavior in a dynamic world.

5.3 Leverage Portfolio Sorts

In a recent article, Lemmon, Roberts and Zender (2008, LRZ) chart the evolution of leverage ratios for four portfolios constructed by sorting firms based on their actual leverage (Figure 1) or unexpected leverage (Figure 2). LRZ report the puzzling evidence that, despite of some convergence, average leverage ratios across the four portfolios are fairly stable over time for both types of sorts (i.e. actual and unexpected leverage). Using the annual COMPUSTAT database for the 1965 to 2003 period, firms with relatively high (low) leverage tend to maintain relatively high (low) leverage for over 20 years. LRZ conclude that the striking stability in leverage paths is unexplained by previously identified determinants (e.g. firm size, profitability, market-to-book, industry, etc.) or changes in sample composition (e.g. firm exit).

In this section, we establish that real frictions in a dynamic trade-off model can produce average leverage paths that closely resemble the corresponding ones documented by LRZ. Put differently, endogenous investment and financing decisions in a dynamic model can largely explain the otherwise puzzling patterns. To this end, we extend the multi-stage model with endogenous financing and investment decisions in Section 2 by introducing an initial coupon, C_0, at beginning of a firm's life. This will enable us to create exogenous variation in initial leverage based on which we can sort firms into leverage portfolios. At time $t = 0$, firms are also endowed with an initial scale, Π_0, so that they can generate cash flows to service their initial debt issues. Given that each firm has debt in place in stage 0, there is also an endogenous default threshold, X_{D0}. The values of initial debt in stages 0, 1, 2 are, respectively, denoted by D_0, D_{10}, and D_{20}. All other variables are the same as in Section 2 (see Appendix A for more details).

We proceed by generating simulated economies for the extended multi-stage model. The panel simulations in this section follow closely the procedure outlined in Section 5.1 with the exception that we now also allow for three different industries based on the structural estimations for subsamples of low, medium, and high Q firms in Section 4. In particular, the sample consists of 3,000

firms over 39 years in 1,000 panel data sets with three industries, which have 1,000 firms each and are defined based on the subsample (i.e. low, medium, high Q) estimation results for b^* in Table 5. Thus, the modeling of firm-level heterogeneity also maintains the assumptions from Section 5.1, except that we replace the SMM's full sample by the SMM's three subsample estimation results. For example, the "Medium Q" industry has investment scales for all firms equal to $\Pi_1 = 2.032$ and $\Pi_2 = 0.848$, the bankruptcy cost, α, and the tax rate, τ, are centered around 0.267 and 0.047, respectively, based on a uniform distribution with ranges of +/–20% around their centers, etc. The initial scale is normalized to one, $\Pi_0 = 1$. Firms have an exogenously assigned initial coupon, C_0, that is drawn from a lognormal distribution with mean 0.5 and variance 1: $C_0 \sim \text{LogNormal}(0.5, 1)$. For each point in time or quarter, $t = 0, ..., 156$, in the simulated economies, we compute book leverage and quasi-market leverage for each firm.[23]

For the simulated data sets, we implement the same procedure as outlined in LRZ for COMPUSTAT data to track average leverage ratios of firms across four portfolios, denoted by "Very Low", "Low", "High" and "Very High," which are based on quartile sorts of these firms' actual leverage. Figure 2 presents the average book and quasi-market leverage ratios for these portfolios in "event time," both for all simulated firms in Panels A and B and for survivors (i.e. firms that exist at least for 20 years) in Panels C and D.[24] As in the real data, firms leave the simulate data because of bankruptcy. In addition, from quarter 76 onward, the length of time for which we can follow each portfolio is censored because we only simulate data for 156 quarters. So, we perform the portfolio formation through quarter 76, which corresponds to 1984 in their sample, for the subsample of firms required to survive for at least 80 quarters (Survivors) in Panels C and D.

[Insert Figure 2 Here.]

The figure shows that average leverage paths for the four portfolios formed as in LRZ converge to stable levels in the long run. However, they do not converge to target leverage, which would be predicted by static trade-off models in which firms always converge to target as soon as they

[23] We find qualitatively identical results if we simulate 139 years and drop the first 100 years or when C_0 obeys e.g. a uniform distribution: $C_0 \sim \text{Uniform}[0.01, 6]$. These unreported results are available from the authors on request.

[24] Each panel presents the average leverage of four portfolios in event time (i.e. quarters), where event time zero is the portfolio formation period. That is, for each quarter in the simulated economies, we form four portfolios by ranking firms based on their actual leverage. Holding the portfolios fixed for the next 20 years, we compute the average leverage for each portfolio. We repeat this process of sorting and averaging for every quarter in the simulated economies. After performing this sorting and averaging for each quarter from quarter 0 to quarter 156, we then average the average leverages across "event time" in each of the simulated economies and then average them across the 1,000 simulated economies to obtain the lines in the figure. We suppress 95% confidence intervals, because they almost coincide with the average leverage lines due to the large scale of the simulations.

make adjustments (or as soon as adjustment costs allow them to do so). Recall that the analysis in Section 3 shows that firms that are otherwise identical (i.e. without considering the structure of investment process) need not have the same target leverage ratios. That is, within the multi-stage model, firms that are otherwise identical (i.e. without considering the structure of investment process) need not follow the same target leverage ratios. Given that the structure of investment process is hard to observe perfectly, the persistence of leverage in Figure 2 therefore means that this unobservable heterogeneity can give the appearance of a transitory or short-term component of debt, even though firms dynamically optimize their permanent or long-term component of debt in our model by trading off bankruptcy costs, tax benefits, and investment benefits.

Furthermore, LRZ point out that a potential concern regarding their main finding is that constructing portfolios based on actual leverage can implicitly pick up cross-sectional variation in underlying factors, which themselves influence cross-sectional variation in leverage, such as bankruptcy costs or industry attributes. Like LRZ, we therefore also form four portfolios by ranking firms based on their "unexpected leverage" and then track again the portfolios' averages of actual leverage in event time. Unexpected leverage is defined as the residuals from a cross-sectional regression of leverage on market-to-book, Q, profitability, π, volatility of cash flows, σ, bankruptcy cost, α, tax rate, τ, firm size, φ, and industry indicator variables, where all independent variables are lagged one year.

Figure 3 presents the evolution of average book and quasi-market leverage ratios in event time for unexpected (instead of actual) leverage portfolios. It reveals that the results are nearly identical to those for actual leverage portfolios in Figure 2. While there is slightly less cross-sectional variation in average leverage, the differences in average leverage across the four portfolios do not quickly disappear in the simulated economies. Thus, unexpected leverage portfolios cannot remove the key variation in C_0 that creates the initial cross-firm differences and then as a result of large enough, real frictions the striking stability in average leverage paths for very long periods of time. So we conclude that persistence is not a special case of some parametrization, simulation, or sorting procedure but rather a general result of the dynamic trade-off model with investment frictions.

[Insert Figure 3 Here.]

In sum, this section implies that the corporate investment process can be the driving force behind leverage ratios' pronounced persistence after long periods of time elapse. To better understand financing dynamics, we thus need to focus more on the heterogeneity in investment dynamics.

6 Conclusion

This paper examines interactions of corporate investment and financing in a dynamic trade-off model with a sequence of irreversible investment opportunities. The model produces an intertemporal effect, which links financial flexibility to the investment process. Firms trade off reaping investment (i.e. cash flow) benefits from issuing debt in an earlier stage against retaining financial flexibility for funding more of the investment cost with debt in a later stage. Taking future financing and investment opportunities into account, (juvenile) firms tend to underutilize debt when financing investment the first time to retain financial flexibility. Surprisingly, the underutilization of debt persists even when the adolescent firm matures (i.e. exercises its last investment opportunity). In addition, underutilization of debt is more (less) severe for the more back-loaded (front-loaded) investment opportunities. That is, even within a standard trade-off model, firms that are identical without considering their investment opportunities do not follow the same target leverage ratios.

Parameter estimation via Simulated Method of Moments takes the model to the real data. Structural estimation results reveal that high growth firms have, on average, a more back-loaded investment process, which helps explain why they tend to have low leverage ratios. Furthermore, capital structure regression results for simulated data using these estimation results produce stylized facts consistent with the empirical literature. Notably, the dynamic trade-off model with a series of endogenous investment and financing decisions is capable of producing a negative leverage-profitability relation and, in the absence of agency problems or other frictions, a negative leverage-growth relation. Therefore, empirical tests without incorporation of the structure of the investment process (and in particular cross-firm variation thereof) are largely uninformative to the extent that their interpretation is not robust to heterogeneity in companies' investment opportunities. Finally, an extension of our dynamic framework to randomly imposed initial variation in leverage at the beginning of the simulated economies reveals that the model can explain the empirical puzzle that average leverage ratios are path-dependent and persistent for very long periods of time.

Overall, we conclude that it is important for studies of capital structure to recognize the structure of the investment process, which strongly influences both investment and financing dynamics. The rather rich set of insights and predictions generated by embedding a sequence of irreversible investments in a dynamic trade-off model suggests that further extension of this class of (real options) models will prove fruitful for future research.

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Appendix A. Extension of the Multi-Stage Model

This appendix presents an extension of the multi-stage model with an initial debt coupon. Let C_0 denote the initial coupon, and Π_0 the scale of the firm in stage 0. As the firm has debt in place in stage 0, there is also an endogenous default threshold is X_{D0}. The values of this initial debt issue in stages 0, 1, 2 are denoted by D_0, D_{10}, and D_{20}. Other variables are the same as in Section 2.

Mature Firm (Stage 2)

In the second stage, the investment options have been exercised, so the firm faces a pure financing decision. The new debt D_{22} is issued in this stage to partially finance the investment cost F_2 and equityholders bear the remainder of the cost. The new debt D_{22} together with the debt issued in the first stage D_{21} and the initial debt D_{20} offers tax savings but creates default risk. The solutions of the debt values are simple generalizations of equation (6). We again assume that D_{22} has the same seniority as D_{21} and D_{20}. The values of the three debt issues for $X \geq X_{D2}$ are given by:

$$\begin{aligned} D_{2i}(X, C_0, C_1, C_2) \;=\; & \frac{C_i}{r}\Big(1 - (\frac{X}{X_{D2}})^a\Big) + \\ & \frac{C_i}{C_0 + C_1 + C_2}\frac{(1-\alpha)(1-\tau)(\Pi_0 + \Pi_1 + \Pi_2)X_{D2}}{r - \mu}(\frac{X}{X_{D2}})^a, \end{aligned} \tag{A.1}$$

where $i = 0, 1, 2$. The value of equity for $X \geq X_{D2}$ can be obtained similarly:

$$\begin{aligned} E_2(X, C_0, C_1, C_2) \;=\; & (1-\tau)\Big(\frac{(\Pi_0 + \Pi_1 + \Pi_2)X}{r - \mu} - \frac{C_0 + C_1 + C_2}{r} - \\ & (\frac{(\Pi_0 + \Pi_1 + \Pi_2)X_{D2}}{r - \mu} - \frac{C_0 + C_1 + C_2}{r})(\frac{X}{X_{D2}})^a\Big). \end{aligned} \tag{A.2}$$

The only decision that the firm's equityholders make in stage 2 is when to default. To maximize the value of this option, equityholders select an endogenous default threshold X_{D2} such that:

$$\frac{\partial E_2(X, C_0, C_1, C_2)}{\partial X}\Big|_{X = X_{D2}} = 0, \tag{A.3}$$

which yields a closed-form solution for the optimal default threshold in the second stage:

$$X_{D2} = \frac{a(C_0 + C_1 + C_2)(r - \mu)}{r(a-1)(\Pi_0 + \Pi_1 + \Pi_2)}. \tag{A.4}$$

Adolescent Firm (Stage 1)

In the first stage, the first investment option has been exercised. The adolescent firm has some assets-in-place and its capital structure is a mix of debt, D_{10} and D_{11}, and equity, E_1. It has both an option to default and an option to invest, so it solves a joint financing and investment problem.

Using similar arguments as in Section 2, each of the valuation equations for D_{10}, D_{11} and E_1 needs to satisfy two boundary conditions. Consider debt $D_{1i}(X, C_0, C_1, C_2)$, with $i = 0, 1$. When $X \downarrow X_{D1}$, equityholders default and debtholders get the liquidation value: $D_{1i}(X_{D1}, C_0, C_1, C_2) = \frac{C_i}{C_0+C_1}\frac{(1-\alpha)(1-\tau)(\Pi_0+\Pi_1)X_{D1}}{r-\mu}$. If the firm keeps growing and X increases to the investment threshold X_{S2}, the firm will exercise the second-stage investment option, and debt values from stage 1 equal debt values in stage 2: $D_{1i}(X_{S2}, C_0, C_1, C_2) = D_{2i}(X_{S2}, C_0, C_1, C_2)$. For $X_{D1} \leq X \leq X_{S2}$, these conditions imply the following solution for debt value in stage 1:

$$\begin{aligned} D_{1i}(X, C_0, C_1, C_2) \;=\; & \frac{C_i}{r}\Big(1 - L(X) - (\frac{X_{S2}}{X_{D2}})^a H(X)\Big) + (1-\alpha)(1-\tau) \\ & \Big(\frac{C_i}{C_0+C_1}\frac{(\Pi_0+\Pi_1)X_{D1}}{r-\mu}L(X) + \\ & \frac{C_i}{C_0+C_1+C_2}\frac{(\Pi_0+\Pi_1+\Pi_2)X_{D2}}{r-\mu}(\frac{X_{S2}}{X_{D2}})^a H(X)\Big), \end{aligned} \tag{A.5}$$

where $i = 0, 1$ and where

$$L(X) \;=\; \frac{X^z X^a_{S2} - X^a X^z_{S2}}{X^z_{D1} X^a_{S2} - X^a_{D1} X^z_{S2}} \tag{A.6}$$

$$H(X) \;=\; \frac{X^z_{D1} X^a - X^a_{D1} X^z}{X^z_{D1} X^a_{S2} - X^a_{D1} X^z_{S2}} \tag{A.7}$$

denote state prices that, respectively, take the value of one if X first reaches the default threshold X_{D1} from above or the investment threshold X_{S2} from below.

The value of equity, E_1, on the other hand, approaches zero when $X \downarrow X_{D1}$. When $X \uparrow X_{S2}$, it satisfies the value-matching condition $E_1(X_{S2}, C_0, C_1, C_2) = E_2(X_{S2}, C_0, C_1, C_2) - [F_2 - D_{22}(X_{S2}, C_0, C_1, C_2)]$ because the fixed investment cost, F_2, is funded by a mix of debt and equity. For $X_{D1} \leq X \leq X_{S2}$, these conditions imply the following solution for equity value in stage 1:

$$\begin{aligned} E_1(X, C_0, C_1, C_2) \;=\; & (1-\tau)\Big[(\frac{(\Pi_0+\Pi_1)X}{r-\mu} - \frac{(C_0+C_1)}{r}) - (\frac{(\Pi_0+\Pi_1)X_{D1}}{r-\mu} - \frac{C_0+C_1}{r})L(X) + \\ & \Big(\frac{\Pi_2 X_{S2}}{r-\mu} - \frac{C_2}{r} - \frac{F_2 - D_{22}(X_{S2}, C_0, C_1, C_2)}{1-\tau} - \\ & (\frac{(\Pi_0+\Pi_1+\Pi_2)X_{D2}}{r-\mu} - \frac{C_0+C_1+C_2}{r})(\frac{X_{S2}}{X_{D2}})^a\Big)H(X)\Big]. \end{aligned} \tag{A.8}$$

The first two terms in equation (A.8) denote the present value of after-tax cash flows to equityholders until the firm defaults in the current stage. The next few terms in this equation show the value from entering into the second stage. Given E_1, equityholders can determine the optimal default threshold, X_{D1}, by maximizing equity value:

$$\frac{\partial E_1(X, C_0, C_1, C_2)}{\partial X}|_{X=X_{D1}} = 0. \tag{A.9}$$

Furthermore, the optimal investment threshold, X_{S2}, solves the smooth-pasting condition:

$$\frac{\partial E_1(X,C_0,C_1,C_2)}{\partial X}|_{X=X_{S2}} = \frac{\partial E_2(X,C_0,C_1,C_2)}{\partial X}|_{X=X_{S2}} + \frac{\partial D_{22}(X,C_0,C_1,C_2)}{\partial X}|_{X=X_{S2}}. \quad \text{(A.10)}$$

Juvenile Firm (Stage 0)

In the initial stage, the juvenile firm now has some assets-in-place, an option on a two-stage investment project, and pre-existing debt. The firm thus faces a joint financing and investment problem. As $X \downarrow X_{D0}$, equityholders default and end up with nothing, $E_0(X_{D0},C_0,C_1,C_2) = 0$, whereas debtholders receive the liquidation value $D_0(X_{D0},C_0,C_1,C_2) = (1-\tau)(1-\alpha)\frac{\Pi_0 X_{D0}}{r-\mu}$. When X touches the first investment threshold X_{S1} the first time from below, the first option is exercised and hence:

$$E_0(X_{S1},C_0,C_1,C_2) \;=\; E_1(X_{S1},C_0,C_1,C_2) - [F_1 - D_{11}(X_{S1},C_0,C_1,C_2)], \quad \text{(A.11)}$$

because debt and equity finance the exercise cost F_1. In addition, the initial debt satisfies the value-matching condition:

$$D_0(X_{S1},C_0,C_1,C_2) \;=\; D_{10}(X_{S1},C_0,C_1,C_2). \quad \text{(A.12)}$$

For $X_{D0} \le X \le X_{S1}$, these conditions yield the following solutions for debt and equity values:

$$\begin{aligned} D_0(X,C_0,C_1,C_2) \;=\; & \frac{C_0}{r}\Big(1-\tilde{L}(X) - [L(X_{S1}) + (\frac{X_{S2}}{X_{D2}})^a H(X_{S1})]\tilde{H}(X)\Big) + \\ & (1-\alpha)(1-\tau)\Big(\frac{\Pi_0 X_{D0}}{r-\mu}\tilde{L}(X) + \frac{C_0}{C_0+C_1}\frac{(\Pi_0+\Pi_1)X_{D1}}{r-\mu}L(X_{S1})\tilde{H}(X) + \\ & \frac{C_0}{C_0+C_1+C_2}\frac{(\Pi_0+\Pi_1+\Pi_2)X_{D2}}{r-\mu}(\frac{X_{S2}}{X_{D2}})^a H(X_{S1})\tilde{H}(X)\Big), \end{aligned} \quad \text{(A.13)}$$

and

$$\begin{aligned} E_0(X,C_0,C_1,C_2) \;=\; & (1-\tau)\Big[(\frac{\Pi_0 X}{r-\mu} - \frac{C_0}{r}) - (\frac{\Pi_0 X_{D0}}{r-\mu} - \frac{C_0}{r})\tilde{L}(X) + \Big((\frac{\Pi_1 X_{S1}}{r-\mu} - \frac{C_1}{r}) - \\ & \frac{F_1 - D_{11}(X_{S1},C_0,C_1,C_2)}{1-\tau} - (\frac{(\Pi_0+\Pi_1)X_{D1}}{r-\mu} - \frac{C_0+C_1}{r})L(X) + \\ & (\frac{\Pi_2 X_{S2}}{r-\mu} - \frac{F_2 - D_{22}(X_{S2},C_0,C_1,C_2)}{1-\tau} - \frac{C_2}{r} - \\ & (\frac{(\Pi_0+\Pi_1+\Pi_2)X_{D2}}{r-\mu} - \frac{C_0+C_1+C_2}{r})(\frac{X_{S2}}{X_{D2}})^a)H(X)\Big)\tilde{H}(X), \end{aligned} \quad \text{(A.14)}$$

where $H(X)$ and $L(X)$ are defined in equation (A.6), and where

$$\tilde{L}(X) \;=\; \frac{X^z X_{S2}^a - X^a X_{S1}^z}{X_{D0}^z X_{S1}^a - X_{D0}^a X_{S1}^z} \quad \text{(A.15)}$$

$$\tilde{H}(X) \;=\; \frac{X_{D0}^z X^a - X_{D0}^a X^z}{X_{D0}^z X_{S1}^a - X_{D0}^a X_{S1}^z} \quad \text{(A.16)}$$

denote state prices that, respectively, take the value of one if X first reaches the default threshold X_{D0} from above or the investment threshold X_{S1} from below.

Finally, the firm's equityholders will choose an optimal pair (C_1, C_2) by maximizing initial firm value subject to the smooth-pasting conditions for X_{D0}, X_{D1}, X_{D2}, X_{S1} and X_{S2} mentioned above:

$$\max_{C_1,C_2} \; D_0(X_0, C_0, C_1, C_2) \; + \; E_0(X_0, C_0, C_1, C_2) \tag{A.17}$$

subject to:

$$\frac{\partial E_0(X, C_0, C_1, C_2)}{\partial X}\Big|_{X=X_{D0}} = 0, \tag{A.18}$$

$$\frac{\partial E_1(X, C_0, C_1, C_2)}{\partial X}\Big|_{X=X_{D1}} = 0, \tag{A.19}$$

$$\frac{\partial E_2(X, C_0, C_1, C_2)}{\partial X}\Big|_{X=X_{D2}} = 0, \tag{A.20}$$

$$\frac{\partial E_0(X, C_0, C_1, C_2)}{\partial X}\Big|_{X=X_{S1}} = \frac{E_1(X, C_0, C_1, C_2)}{X}\Big|_{X=X_{S1}} + \frac{D_{11}(X, C_0, C_1, C_2)}{X}\Big|_{X=X_{S1}}, \tag{A.21}$$

$$\frac{\partial E_1(X, C_0, C_1, C_2)}{\partial X}\Big|_{X=X_{S2}} = \frac{E_2(X, C_0, C_1, C_2)}{X}\Big|_{X=X_{S2}} + \frac{D_{22}(X, C_0, C_1, C_2)}{X}\Big|_{X=X_{S2}}. \tag{A.22}$$

Appendix B. Simulated Method of Moments

We estimate the structural parameters of the model via Simulated Method of Moments (SMM), which is based on indirect inference techniques in Gourieroux, Monfort, and Renault (1993) and Gourieroux and Monfort (1996). By varying the vector of model parameters, b, SMM minimizes the distance between model moments, denoted as $M_m(b)$, and data moments, denoted as M_d. Note that we explicitly state the dependence of the simulated moments, $M_m(b)$, on the vector of structural parameter values, b.

The simulated moments parameter estimation procedure can be summarized as follows (see e.g. Hennessy and Whited (2005, 2007) or Strebulaev and Whited (2012) for further details):

1. We first compute N_d data moments from COMPUSTAT to generate the vector of data moments, M_d. We use fixed firm and year effects in the estimation of all of our data moments to remove heterogeneity from the actual data.

2. The inverse covariance matrix of the data moments yields the optimal weighting matrix:

$$W_d \;=\; [N_d \mathrm{Var}(M_d)]^{-1}\,, \tag{B.1}$$

   which places more weight on more precisely measured moments. Reliance on the influence-function approach in Erickson and Whited (2000) yields qualitatively identical results.

3. For each vector of structural parameter values, b, we simulate a set of S panel data sets with i.i.d. firms each containing $2 * T$ firm-year observations. We discard the first T years of data to avoid non-stationarity and other problems arising from the initial conditions of the simulations. We then calculate the same set of moments as in step 1 using our S simulated panel data sets to generate $M_m(b)$.

4. We then calculate the weighted distance between the model moments and the data moments:

$$J_{N_d}(b) \;=\; \Big[M_d - \frac{1}{S}\sum_{i=1}^{S} M_m(b)\Big]' W_d \Big[M_d - \frac{1}{S}\sum_{i=1}^{S} M_m(b)\Big], \tag{B.2}$$

   where W_d is the positive definite weighting matrix from step 2.

5. Finally, by varying b iteratively, we find an optimal set of structural parameter values, b^*, which minimizes the objective function, $J_{N_d}(b)$:

$$b^* \;=\; \arg\min_b \Big[M_d - \frac{1}{S}\sum_{i=1}^{S} M_m(b)\Big]' W_d \Big[M_d - \frac{1}{S}\sum_{i=1}^{S} M_m(b)\Big]. \tag{B.3}$$

Table 1. Description of Model Parameters and Variables

This table presents a notion index for the single-stage (benchmark) model and the multi-stage model.

Parameter	Definition
r	Risk-free interest rate
μ	Growth rate of cash flows
σ	Volatility of cash flows
τ	Effective corporate tax rate
α	Proportional bankruptcy cost
X_0	Cash flow level (in \$) at time $t = 0$
Π_i, Π	Investment scale of ith stage, $i = 1, 2$
F_i, F	Investment cost (in \$) of ith stage, $i = 1, 2$
C_i, C	Debt coupon (in \$) of ith stage, $i = 1, 2$
X_{Si}, X_S	Investment threshold of ith stage, $i = 1, 2$
X_{Di}, X_D	Default threshold of ith stage, $i = 1, 2$
D_B	Debt value in stage 1 of the benchmark model
D_1	Debt value in stage 1 of the multi-stage model
D_{2i}	Debt value in stage 2 of the multi-stage model, $i = 1, 2$
E_{Bi}	Equity value in stage i of the benchmark model, $i = 0, 1$
E_i	Equity value in stage i of the multi-stage model, $i = 0, 1, 2$
ML_i, ML	Market leverage in ith stage, $i = 1, 2$

Table 2. Financing and Investment in Single-Stage and Multi-Stage Models

This table shows the optimal investment and financing decisions of the single-stage benchmark model in Panel A and the multi-stage model in Panel B. The base case parameter values are as follows: risk-free rate $r = 6\%$, growth rate of the cash flow process $\mu = 1\%$, volatility of the cash flow process $\sigma = 25\%$, corporate tax rate $\tau = 10\%$, bankruptcy cost $\alpha = 30\%$, initial value of the cash flow process $X_0 = \$5$, the scales of investment $\Pi_1 = 1$ and $\Pi_2 = 1$, and the investment costs $F_1 = \$100$ and $F_2 = \$200$. The notation index is given in Table 1.

Panel A. Single-Stage Model

	$\Pi = 1$ $F = \$100$	$\Pi = 1$ $F = \$200$	$\Pi = 1.5$ $F = \$100$	$\Pi = 0.5$ $F = \$200$
C	6.522	13.034	6.521	13.034
X_S	12.487	24.973	8.325	49.947
X_D	2.830	5.657	1.887	11.313
ML	0.419	0.419	0.419	0.419

Panel B. Multi-Stage Model

	$\Pi_1 = 1$ $\Pi_2 = 1$	$\Pi_1 = 0.75$ $\Pi_2 = 1.25$	$\Pi_1 = 1.25$ $\Pi_2 = 0.75$	$\Pi_1 = 1.5$ $\Pi_2 = 0.5$
C_1	5.591	5.447	5.972	6.261
C_2	19.428	14.760	27.205	43.219
X_{S1}	12.364	16.424	9.930	8.300
X_{S2}	23.666	19.359	30.764	44.611
X_{D1}	2.154	2.477	1.959	1.770
X_{D2}	5.429	4.385	7.199	10.737
ML_1	0.283	0.201	0.349	0.390
ML_2	0.378	0.401	0.359	0.343

Table 3. Sensitivity of Financing and Investment

This table shows comparative statics of parameters unrelated to the investment process. The base case parameter values are as follows: risk-free rate $r = 6\%$, growth rate of the cash flow process $\mu = 1\%$, volatility of the cash flow process $\sigma = 25\%$, corporate tax rate $\tau = 10\%$, bankruptcy cost $\alpha = 30\%$, initial value of the cash flow process $X_0 = \$5$, the scales of investment $\Pi_1 = 1$ and $\Pi_2 = 1$, and the investment costs $F_1 = \$100$ and $F_2 = \$200$. Relative to the base case, we increase or decrease a parameter by 50% while keeping everything else fixed. The notation index is given in Table 1.

	Base	$\tau = 15\%$	$\tau = 5\%$	$\alpha = 45\%$	$\alpha = 15\%$	$\sigma = 37.5\%$	$\sigma = 12.5\%$	$\mu = 1.5\%$	$\mu = 0.5\%$
C_1	5.591	7.427	3.312	4.648	6.766	5.352	5.802	6.084	5.197
C_2	19.428	24.580	12.265	15.603	25.630	25.130	17.364	21.424	17.822
X_{S1}	12.364	12.640	12.004	12.450	12.223	17.509	8.498	11.989	12.745
X_{S2}	23.666	23.677	23.601	24.233	22.521	33.083	16.456	22.908	24.441
X_{D1}	2.154	2.781	1.324	1.819	2.553	1.360	3.447	2.099	2.201
X_{D2}	5.429	6.945	3.380	4.394	7.030	4.711	7.187	5.517	5.348
ML_1	0.283	0.336	0.198	0.250	0.319	0.153	0.533	0.271	0.296
ML_2	0.378	0.445	0.268	0.324	0.451	0.290	0.528	0.380	0.376

Table 4. Sensitivity of Model Moments

This table presents the sensitivities of the moments used in the Simulated Method of Moments (SMM) estimation. The structural model parameters that we fit by SMM are the investment scales, Π_1 and Π_2, the bankruptcy cost, α, and the tax rate, τ. The other parameters assume the base case values from Table 2. Column 1 presents the model moments for the base case (i.e. $\Pi_1 = 1$, $\Pi_2 = 1$, $\alpha = 0.3$, and $\tau = 0.1$). In columns 2 to 5, each parameter is increased by 50% while keeping the others fixed. The following five moments are used in the SMM. The average quasi-market leverage, QML, is obtained by first calculating cross-sectional averages of quasi-market leverage ratios for every time t and then averaging across time. Quasi-market leverage is defined as the book value of debt divided by the sum of market value of equity and book value of debt. The dispersion of quasi-market leverage ratios, $DispQML$, is the cross-sectional average of the time-series standard deviations of firms' quasi-market leverage ratios. D/K denotes net debt issuance normalized by capital. D/K is calculated only at the investment points. Q is the average market-to-book ratio. Similar to QML, the average is taken first across firms and then across time. Inv/Eq is the average of investment expenditure scaled by the book value of equity at investment points. Panel A displays the sensitivities of the model moments in terms of their absolute changes, while Panel B displays their changes relative to the base case values in the first column of Panel A.

Panel A. Absolute Changes

	Base	$\Pi_1 = 1.5$	$\Pi_2 = 1.5$	$\alpha = 45\%$	$\tau = 15\%$
QML	0.064	0.115	0.064	0.067	0.057
$DispQML$	0.070	0.107	0.070	0.072	0.065
D/K	0.267	0.305	0.231	0.221	0.337
Q	1.184	1.335	1.678	1.190	1.139
Inv/Eq	0.413	0.427	0.394	0.405	0.432

Panel B. Relative Changes

	$\Pi_1 = 1.5$	$\Pi_2 = 1.5$	$\alpha = 45\%$	$\tau = 15\%$
QML	0.805	0.008	0.057	-0.105
$DispQML$	0.527	0.001	0.027	-0.064
D/K	0.140	-0.135	-0.172	0.260
Q	0.128	0.418	0.005	-0.038
Inv/Eq	0.033	-0.048	-0.020	0.046

Table 5. Estimation of Model Parameters with Simulated Method of Moments

This table presents the estimation results of the model parameters via Simulated Method of Moments (SMM). The structural model parameters that we fit by SMM are the investment scales, Π_1 and Π_2, the bankruptcy cost, α, and the tax rate, τ. The other parameters assume the base case values from Table 2. The following five moments are used in the SMM. The average quasi-market leverage, QML, is obtained by first calculating cross-sectional averages of quasi-market leverage ratios for every time t and then averaging across time. Quasi-market leverage is defined as the book value of debt divided by the sum of market value of equity and book value of debt. The dispersion of quasi-market leverage ratios, $DispQML$, is the cross-sectional average of the time-series standard deviations of firms' quasi-market leverage ratios. D/K denotes net debt issuance normalized by capital. D/K is calculated only at the investment points. Q is the average market-to-book ratio. Similar to QML, the average is taken first across firms and then across time. Inv/Eq is the average of investment expenditure scaled by the book value of equity at investment points. The data moments are calculated using COMPUSTAT's annual tapes for the 1965–2009 period. Four sets of data moments are obtained by using the full sample and three subsamples, which are generated by the tercile cutoffs of Q. Panel A presents the fitted model parameters. The numbers in parentheses are the standard deviation of the fitted parameters b^* across the iterations of SMM with the exception of the χ^2 column in Panel A, in which the numbers in parentheses are the p-values for the overidentification test. Panel B presents the target and fitted moments for each sample.

Panel A. Parameter Estimates

		Π_1	Π_2	α	τ	χ^2
Full Sample	b^*	1.966	1.286	0.324	0.043	0.021
		(0.104)	(0.095)	(0.055)	(0.012)	(0.111)
Low Q	b^*	3.036	0.531	0.440	0.039	0.034
		(0.503)	(0.389)	(0.018)	(0.003)	(0.146)
Medium Q	b^*	2.032	0.848	0.267	0.047	0.036
		(0.134)	(0.144)	(0.091)	(0.015)	(0.133)
High Q	b^*	1.264	2.887	0.284	0.071	0.035
		(0.079)	(0.402)	(0.104)	(0.030)	(0.132)

Panel B. Fitted and Data Moments

		QML	$DispQML$	D/K	Q	Inv/Eq
Full Sample	Data	0.199	0.183	0.166	1.685	0.366
	Fitted	0.198	0.157	0.166	1.761	0.412
Low Q	Data	0.290	0.198	0.126	0.905	0.336
	Fitted	0.284	0.207	0.134	1.054	0.407
Medium Q	Data	0.216	0.169	0.210	1.335	0.373
	Fitted	0.220	0.165	0.224	1.403	0.420
High Q	Data	0.087	0.108	0.176	2.839	0.390
	Fitted	0.086	0.086	0.189	2.731	0.394

Table 6. Parameters for Simulation and Descriptive Statistics of Simulated Data

This table presents the parameter values and distributions used for the simulation in Panel A and the descriptive statistics of the simulated leverage ratios in Panel B. To add heterogeneity to the simulated data, several model parameters are randomized at time 0 and kept fixed over time: the investment costs, F_1 and F_2, the bankruptcy cost, α, and the tax rate, τ. In addition, to allow for a correlation structure, the volatility of cash flows is decomposed into a systematic part, σ_S, and an idiosyncratic part, σ_I. β measures a firm's exposure to systematic risk. The investment scales, Π_1 and Π_2, and the means of the bankruptcy cost, α, and the tax rate, τ, are set to the full sample SMM estimates for b^* in Table 5. The other parameters assume the base case values from Table 2. Panel B reports the distributions of market leverage (ML) and quasi-market leverage (QML). Investment points (Inv. Pts.) refers to the data points where firms are at their investment points. Investment points are further classified as the first and second investment points because there are two stages in the model. All other statistics are given for all data points (i.e. in dynamics). The market leverage ratio, ML, is defined as the market value of debt over the sum of market value of debt and market value of equity, and the quasi-market leverage ratio, QML, is the book value of debt over the sum of market value of equity and book value of debt. For each leverage ratio, the mean, the 1st, 5th, 10th, 50th, 90th, 95th, 99th percentiles, and the standard deviation are reported. For each data set, the statistics are first calculated for each quarter, then averaged across quarters, and then averaged across simulated data sets. Min. and Max. give the minimum and maximum of statistics over the 1,000 data sets. The statistics are based on 1,000 simulated economies, which each contain 400 quarters (after dropping the first 400 quarters) for 3,000 firms.

Panel A. Model Parameters for Simulation

Parameter	Value	Parameter	Distribution
Π_1	2.093	F_1	Uniform[80, 120]
Π_2	1.304	F_2	Uniform[160, 240]
σ_S	0.148	α	Uniform[0.362, 0.542]
N	3,000	τ	Uniform[0.022, 0.032]
Δt	0.25	β	Uniform[0.179, 1.807]
T	100	σ_I	$0.05 + \frac{1}{30}\chi^2(5)$

Panel B. Descriptive Statistics for Leverage

		Percentiles							
	Mean	1%	5%	10%	50%	90%	95%	99%	Std. Dev.
ML									
Inv. Pts.	0.187	0.023	0.046	0.067	0.175	0.323	0.368	0.462	0.099
1st Inv. Pts.	0.162	0.021	0.039	0.057	0.152	0.283	0.318	0.386	0.086
2nd Inv. Pts.	0.237	0.042	0.080	0.109	0.225	0.380	0.426	0.521	0.106
Avg.	0.197	0.000	0.000	0.000	0.089	0.571	0.707	0.899	0.241
Min.	0.113	0.000	0.000	0.000	0.000	0.362	0.503	0.784	0.174
Max.	0.255	0.000	0.000	0.000	0.181	0.698	0.833	0.960	0.285
QML									
Avg.	0.205	0.000	0.000	0.000	0.088	0.606	0.752	0.933	0.254
Min.	0.116	0.000	0.000	0.000	0.000	0.378	0.538	0.838	0.185
Max.	0.266	0.000	0.000	0.000	0.182	0.747	0.876	0.977	0.299

Table 7. Capital Structure Regressions on Simulated Data

This table reports average coefficient estimates and average t-statistics (in parentheses) of four cross-sectional regressions over the 1,000 simulated panel data sets from Table 6. That is, the regressions are based on 1,000 simulated economies, which each contain 400 quarters (after dropping the first 400 quarters) for 3,000 firms. The regression model is as follows:

$$QML_i = \beta_0 + \beta_1\, x_i + \beta_2\, \sigma_i + \beta_3\, \alpha_i + \beta_4\, \tau_i + \beta_4\, \varphi_i + \epsilon_i, \tag{B.4}$$

where x is either profitability, π, in Panel A or market-to-book, Q, in Panel B. In Panel C, we include both profitability, π, and market-to-book, Q, as regressors. We measure profitability, π, as earnings before interest and tax (or cash flows) scaled by total assets, whereas the market-to-book ratio, Q, is the ratio of total market value of asset over book value of asset. The other independent variables are constant firm attributes. They include volatility of cash flows, σ, bankruptcy cost, α, tax rate, τ, and firm size, φ, which equals the sum of book value of debt and book value of equity. The first column (Inv. Pts.) shows OLS regression results using data at investment points only. The regressions in the other columns are for all data points (i.e. in dynamics). The second column (BJK) reports OLS regression results in the fashion of Bradley, Jarrel, and Kim (1984). The dependent variable, QML_i, is calculated as the sum of book values of debt over the 400 quarters divided by the sum of book values of debt and market values of equity over the 400 quarters. The independent variables are calculated similarly (if possible). This definition implies that the dependent variable and independent variables are contemporaneous. The third column (RZ) follows Rajan and Zingales (1995), who define all independent variables as averages over quarters $t-1$ to $t-4$. In this version, the dependent variable QML_i is measured at time t. The last column (FF) adopts the Fama-MacBeth regression approach as in Fama and French (2002). At each time t, QML is regressed on lagged independent variables. Then the time-series of the coefficient estimates are averaged and the standard errors are corrected using the Newey-West method with six lags.

Panel A. Profitability

	Inv. Pts.	BJK	RZ	FF
Constant	0.293	0.371	0.323	0.364
	(18.67)	(12.20)	(6.40)	(47.45)
π	2.208	-0.053	-0.004	-0.012
	(10.25)	(-11.04)	(-5.46)	(-11.83)
σ	-0.791	-0.779	-0.754	-0.843
	(-52.55)	(-30.94)	(-18.03)	(-48.66)
α	-0.328	-0.176	-0.097	-0.107
	(-14.43)	(-2.77)	(-0.94)	(-10.57)
τ	2.785	1.427	0.707	0.775
	(16.40)	(3.00)	(0.92)	(10.06)
φ	0.028	0.067	0.184	0.182
	(7.45)	(8.14)	(18.93)	(27.62)
R^2	0.804	0.313	0.229	0.224
N	2,637	3,000	3,000	1,197,000

Panel B. Tobin's Q

	Inv. Pts.	BJK	RZ	FF
Constant	0.369	0.403	0.430	0.471
	(38.06)	(14.10)	(9.02)	(59.55)
Q	0.026	-0.049	-0.076	-0.084
	(28.90)	(-20.17)	(-20.23)	(-32.85)
σ	-0.945	-0.937	-1.072	-1.152
	(-112.52)	(-37.49)	(-25.65)	(-66.97)
α	-0.338	-0.208	-0.128	-0.136
	(-16.67)	(-3.49)	(-1.31)	(-14.37)
τ	2.892	1.679	0.916	0.966
	(19.16)	(3.77)	(1.26)	(13.58)
φ	0.033	0.167	0.265	0.259
	(9.93)	(19.96)	(27.95)	(36.20)
R^2	0.844	0.405	0.344	0.233
N	2,637	3,000	3,000	1,197,000

Panel C. Profitability and Tobin's Q

	Inv. Pts.	BJK	RZ	FF
Constant	0.212	0.423	0.444	0.485
	(15.20)	(15.21)	(9.39)	(59.39)
π	3.162	-0.058	-0.005	-0.015
	(16.43)	(-13.08)	(-7.34)	(-11.96)
Q	0.025	-0.052	-0.079	-0.088
	(25.46)	(-21.57)	(-20.95)	(-33.27)
σ	-0.805	-0.958	-1.088	-1.161
	(-58.13)	(-39.36)	(-26.25)	(-67.00)
α	-0.333	-0.208	-0.129	-0.136
	(-17.70)	(-3.59)	(-1.33)	(-14.44)
τ	2.752	1.681	0.924	0.980
	(19.57)	(3.89)	(1.28)	(13.76)
φ	0.065	0.157	0.259	0.252
	(9.28)	(19.11)	(27.48)	(36.01)
R^2	0.866	0.439	0.357	0.240
N	2,637	3,000	3,000	1,197,000

Figure 1. Initial Equity Values as a Function of Debt Coupon Choices

This figure charts the intertemporal effect by mapping debt coupon pairs (C_1, C_2) into initial equity value, E_0, on the basis of equation (16). C_1 varies from \$4 to \$7, and C_2 from \$16 to \$22. The base case parameter values are as follows: risk-free rate $r = 6\%$, growth rate of the cash flow process $\mu = 1\%$, volatility of the cash flow process $\sigma = 25\%$, corporate tax rate $\tau = 10\%$, bankruptcy cost $\alpha = 30\%$, initial value of the cash flow process $X_0 = \$5$, the scales of investment $\Pi_1 = 1$ and $\Pi_2 = 1$, and the investment costs $F_1 = \$100$ and $F_2 = \$200$.

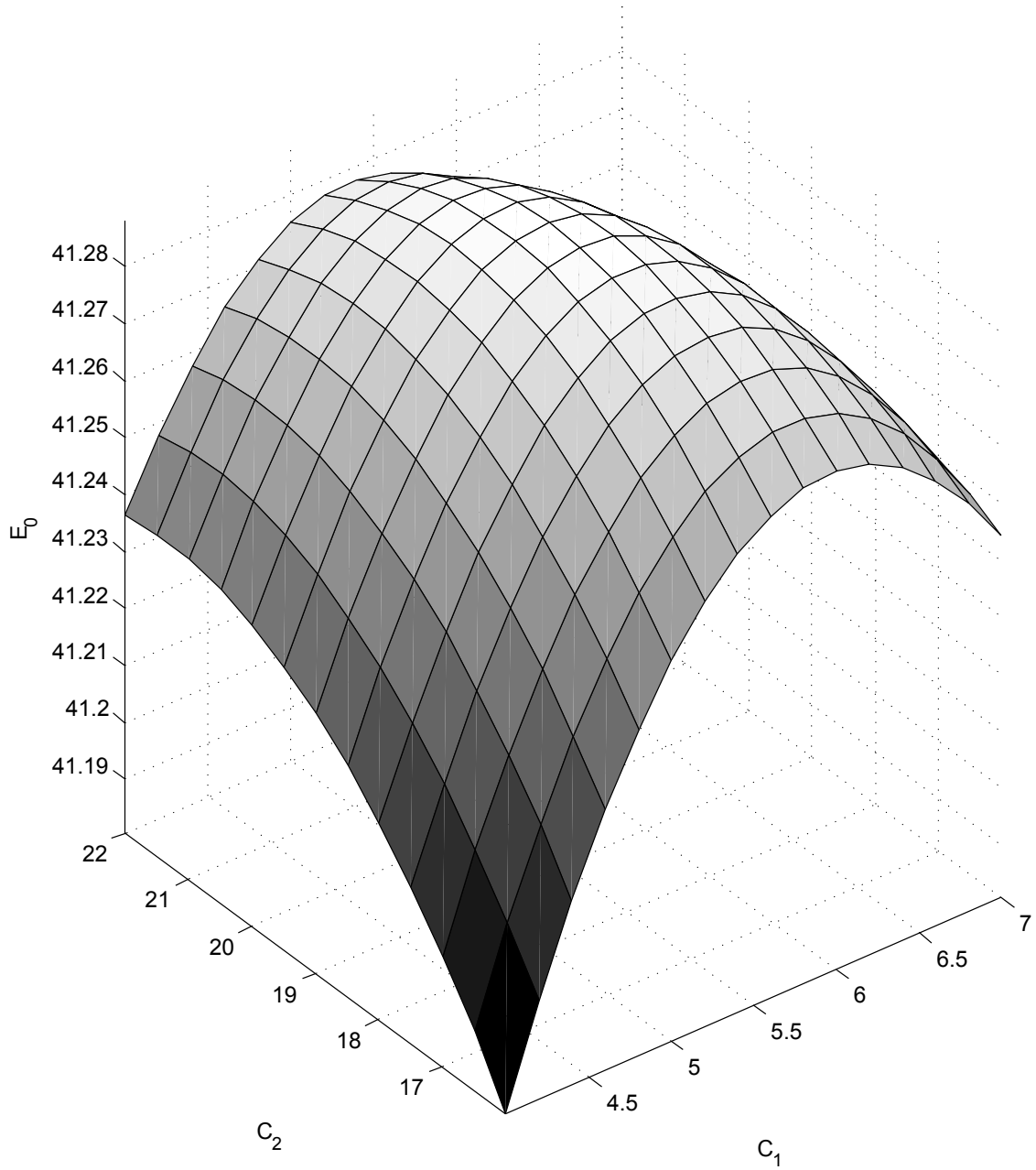


Figure 2. Average Leverage of Actual Leverage Portfolios in Event Time

The sample consists of 3,000 firms over 39 years in 1,000 simulated economies based on the extended multi-stage model in Appendix A with three industries, which have 1,000 firms each and are defined based on the subsample (i.e. low, medium, high Q) estimation results for b^* in Table 5. The modeling of firm-level heterogeneity follows the procedure in Table 6, except that we use here the three subsample estimation results for b^* in Table 5. While the initial investment scale is normalized to one, $\Pi_0 = 1$, firms have an exogenously assigned initial coupon, C_0, which is drawn from a lognormal distribution: $C_0 \sim \text{LogNormal}(0.5, 1)$. Each panel presents the average leverage of four portfolios in event time (i.e. quarters), where event time zero is the portfolio formation period. That is, for each quarter in the simulated economies, we form four portfolios by ranking firms based on their actual leverage. Holding the portfolios fixed for the next 20 years, we compute the average leverage for each portfolio. We repeat this process of sorting and averaging for every quarter in the simulated economies. After performing this sorting and averaging for each quarter from quarter 0 to quarter 156, we then average the average leverages across "event time" in each of the simulated economies and then average them across the 1,000 simulated economies to obtain the lines in the figure. The results for book and quasi-market leverage are presented in Panels A and C, where book (quasi-market) leverage is defined as the ratio of book value of debt to book value of assets (sum of book value of debt and market value of equity). Panels B and D present similar results for book and quasi-market leverage, respectively, but for a subsample of firms required to exist for at least 80 quarters (consequently, we can only perform the portfolio formation through quarter 76 for this sample).

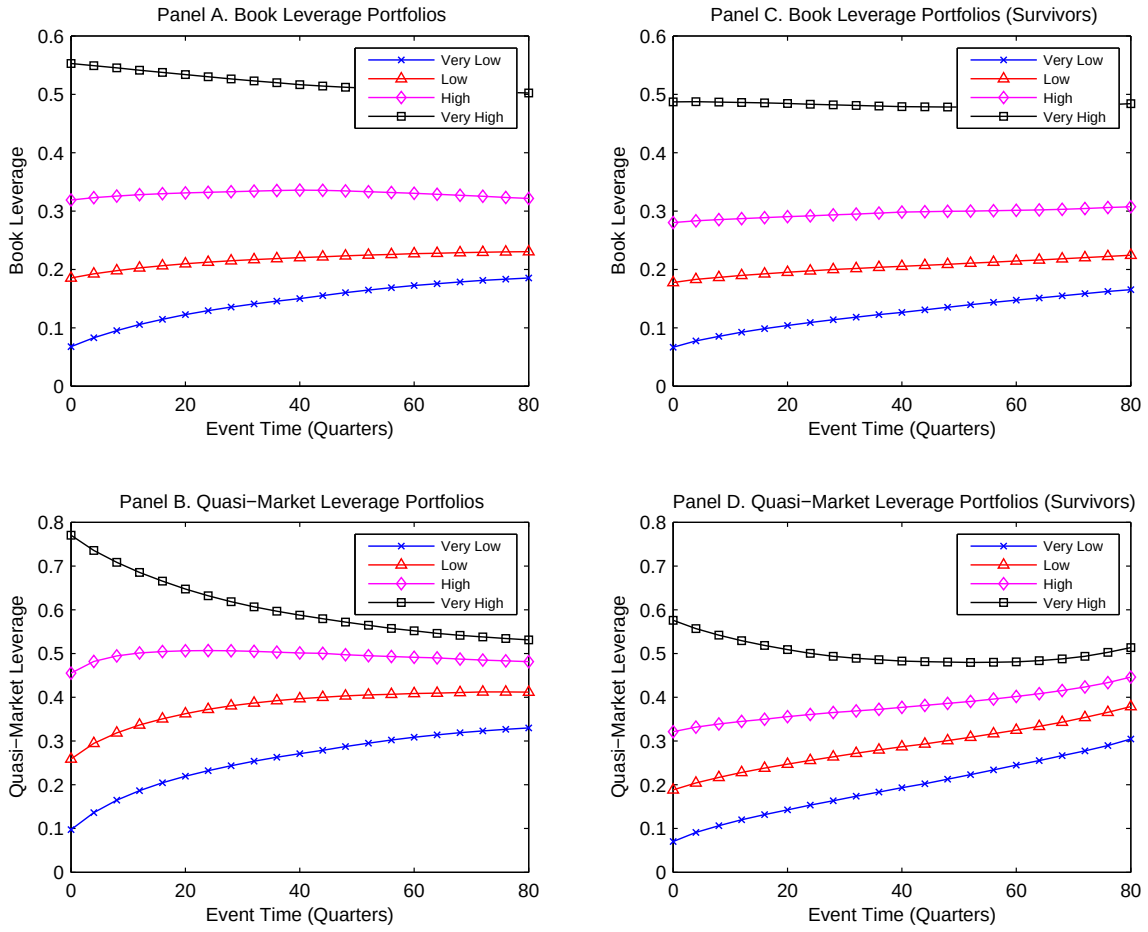
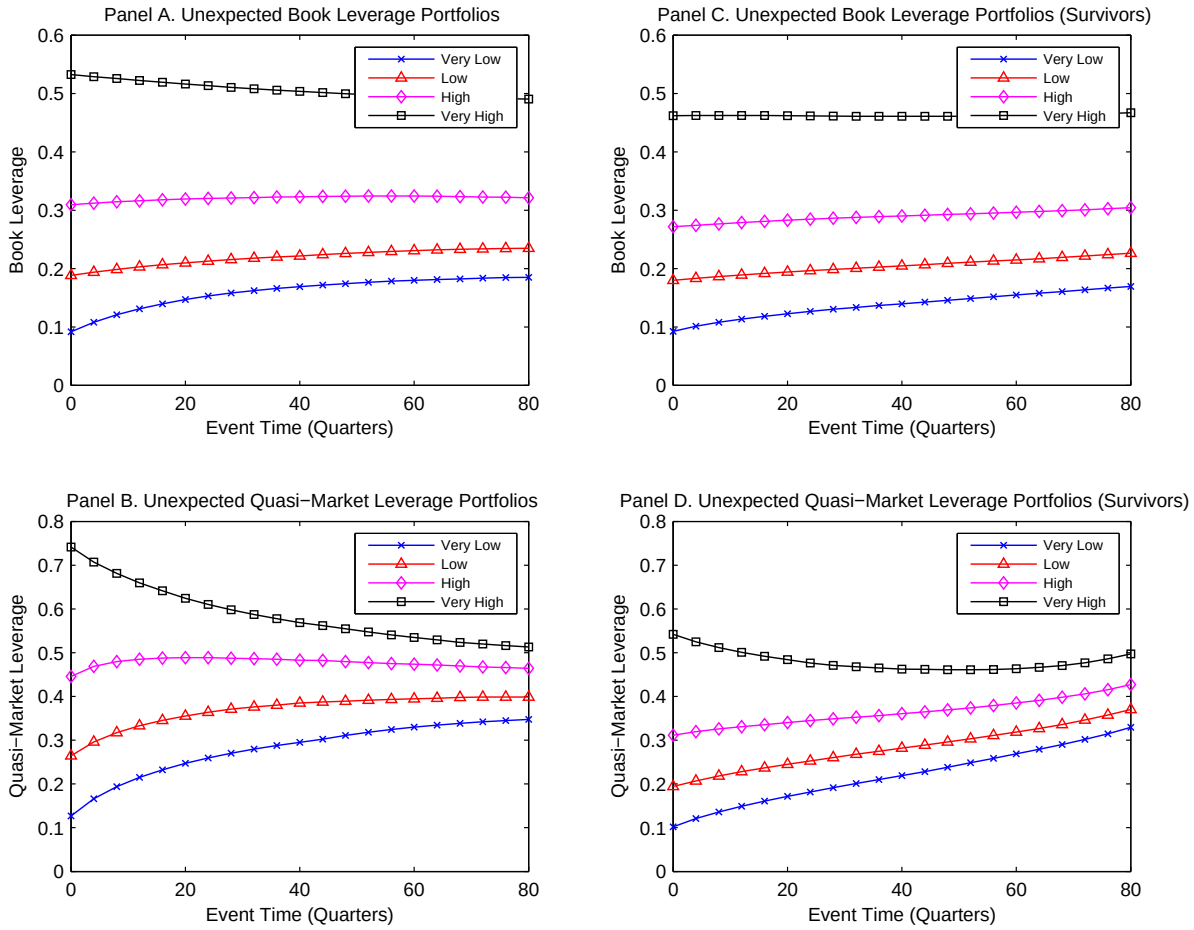


Figure 3. Average Leverage of Unexpected Leverage Portfolios in Event Time.

The sample consists of 3,000 firms over 39 years in 1,000 simulated economies based on the extended multi-stage model in Appendix A with three industries, which have 1,000 firms each and are defined based on the subsample (i.e. low, medium, high Q) estimation results for b^* in Table 5. The modeling of firm-level heterogeneity follows the procedure in Table 6, except that we use here the three subsample estimation results for b^* in Table 5. While the initial investment scale is normalized to one, $\Pi_0 = 1$, firms have an exogenously assigned initial coupon, C_0, which is drawn from a lognormal distribution: $C_0 \sim \text{LogNormal}(0.5, 1)$. Each panel presents the average leverage of four portfolios in event time (i.e. quarters), where event time zero is the portfolio formation period. That is, for each quarter in the simulated economies, we form four portfolios by ranking firms based on their unexpected leverage (defined below). Holding the portfolios fixed for the next 20 years, we compute the average leverage for each portfolio. We repeat this process of sorting and averaging for every quarter in the simulated economies. After performing this sorting and averaging for each quarter from quarter 0 to quarter 156, we then average the average leverages across "event time" in each of the simulated economies and then average them across the 1,000 simulated economies to obtain the lines in the figure. The results for book and quasi-market leverage are presented in Panels A and C, where book (quasi-market) leverage is defined as the ratio of book value of debt to book value of assets (sum of book value of debt and market value of equity). Panels B and D present similar results for book and quasi-market leverage, respectively, but for a subsample of firms required to exist for at least 80 quarters (consequently, we can only perform the portfolio formation through quarter 76 for this sample). Unexpected leverage is defined as the residuals from a cross-sectional regression of leverage on market-to-book, Q, profitability, π, volatility of cash flows, σ, bankruptcy cost, α, tax rate, τ, firm size, φ, and industry indicator variables, where all independent variables are lagged one year.