

Autoencoder-Based Risk-Neutral Model for Interest Rates

Andrei Lyashenko¹, Fabio Mercurio² and Alexander Sokol³

¹*Quantitative Risk Management, Inc.*

²*Bloomberg, L.P.* *

³*CompatibL*

May 22, 2024

Abstract

It is well known that yield curves have low effective dimensionality, and can be accurately represented using very few latent variables. The recent extension to non-linear representations by means of autoencoders (AE) provided further improvement in accuracy compared to the classical linear representations from the Nelson-Siegel family or those obtained using principal component analysis (PCA). We examine Q-measure dynamics in an economy where historical curve evolution is consistent with such low dimensional representations (manifolds) and describe the constraints under which instrument prices in this economy can be arbitrage free for any level of volatility. We then derive the most general form of such arbitrage-free manifolds, and propose a new approach to constructing them based on the geometric concept of “generating manifolds”. In conclusion, we present a Q-measure model based on arbitrage-free AE manifolds and discuss theoretical and practical benefits of the proposed approach for risk and pricing applications.

*The views and opinions expressed in this article are our own and do not represent the opinions of any firm or institution. Bloomberg LP and Bloomberg Professional service are trademarks and service marks of Bloomberg Finance L.P., a Delaware limited partnership, or its subsidiaries. All rights reserved.

Contents

1	Introduction	3
2	Autoencoder-Based State Variable Selection	4
3	Curve Parameterization	5
4	Time Shift Invariance and Static Arbitrage	6
5	Stationarity of the Long Forward Rate	7
6	Arbitrage-Free Interpolation	8
7	Forward Rate Manifold	9
8	Linear Manifold Construction	10
9	Nonlinear Manifold Construction	12
10	Risk-Neutral Model	16
11	Linear Manifolds and Short Rate Models	18
12	Conclusion	19
	References	21
	Appendices	21
A	Proof for the Linear Case	22
A.1	Diagonalizable Generating Matrix	22
A.2	Non-Diagonalizable Generating Matrix	23

1 Introduction

Classical risk-neutral pricing theory holds that complex instruments that do not have their own market-based price discovery mechanism can be priced by calibrating a risk-neutral (Q-measure) model to the prices of simpler instruments that do. The Q-measure (risk-neutral) probabilities of market scenarios in such pricing model are different from their P-measure (real-world) probabilities because of the risk premium. The pivotal insight by Black, Scholes and Merton [1, 2] that constructing a Q-measure model from liquid prices does not require estimation of P-measure probabilities is the foundation of modern derivatives pricing.

The derivation of risk-neutral valuation principle assumes the existence of an idealized frictionless market where a complete set of liquid instruments is available to set up dynamic hedging for every source of risk of the instrument being priced. In such idealized market, the question of whether or not such Q-measure model generates market scenarios that can occur in the real-world is irrelevant as the model only performs interpolation between liquid market prices. According to the risk-neutral pricing theory, the properties of market scenarios in such idealized market are incorporated into the Q-measure pricing model through their effect on the prices of liquid instruments, eliminating the need to make them a direct model input.

Practitioners are well aware that real financial markets fall far short of the idealized conditions described in the preceding paragraph. For the vast majority of instruments, not every source of financial risk can be hedged (incomplete markets). But even if every relevant hedging instrument existed, calibrating the model to all of them would cause pricing instability due to the market noise and liquidity effects (friction). As a result, many pricing models require the use of parameters, such as instantaneous correlations of the model's risk drivers, that cannot be implied from price data and must be estimated historically, and subsequently kept fixed within the model to avoid price and risk instabilities.

Instead of using such poor measure of curve interdependence as correlations, our goal is to construct a model that reflects the reliable historical patterns of dependence between different yield curve points. A Q-measure model that respects such historical dependence structure is, by construction, more likely to produce realistic, stable, and less costly hedges.

In this paper, we describe an approach to Q-measure model construction that captures the dependence structure of interest rates using autoencoders, which are algorithms designed to optimally represent a high-dimensional dataset, in our case historical interest rates across all maturities, using a small number of latent variables. When these latent variables are used as state variables of a Q-measure model, they make the model both consistent with historical interest rate patterns and capable of traditional calibration to market-implied prices. Our model is constructed so as to exclude future curve shapes that are unlikely to occur in practice, and to provide the best possible approximation to historically observed shapes given the chosen number of state variables.

The rest of the paper is organized as follows. Section 2 describes the concept of dimension reduction using autoencoders. Section 3 introduces the relevant notation, which involves parameterizing the curve using time to maturity rather than absolute maturity as per standard convention. In Sections 4, 5, and 6 we derive the conditions required for our

curve representation to be free of static arbitrage. We then introduce the concept of static arbitrage-free forward rate manifold in Section 7 and describe construction of linear manifolds in Section 8 and Appendix A and nonlinear manifolds in Section 9. We present a risk-neutral model based on the arbitrage-free manifolds in Section 10 and discuss a connection to the multi-factor Gaussian short rate models in Section 11. We conclude the paper by discussing the practical applications of the proposed model in Section 12.

We note that such order of presentation follows a somewhat unconventional approach. Instead of postulating model dynamics at the beginning, we present a constructive step-by-step procedure where the proposed stochastic process naturally follows from a series of assumptions and results toward achieving a specific model property, i.e., ensuring that curve shapes generated by the model are broadly similar to the historically observed shapes.

2 Autoencoder-Based State Variable Selection

Properties of an interest rate model are to a large extent determined by the choice of its state variables. Having too many causes parameter estimation issues and negatively affects the performance of certain numerical methods such as American Monte Carlo. Having too few or choosing them poorly causes the model to misprice relevant market instruments or miss certain risks. The optimal number of state variables allows the model to capture hedgeable sources of risk while preserving historical patterns of market movements. This is why dimension reduction, i.e., decreasing the number of state variables with the least possible loss of accuracy, is of paramount importance.

Dimension reduction for a yield curve is a compression algorithm, not unlike those used to compress an image. Each uncompressed raw image is a point in high dimensional space that consists of three dimensions per pixel representing red, green and blue color intensities. A compressed image uses lower-dimensional space and therefore takes fewer bits to store. While storage space is not a consideration in interest rate modelling, faithfully representing the curve using a small number of well-chosen state variables is, and we can leverage the algorithms originally developed for image compression for this purpose.

Reducing image resolution (i.e. the number of pixels) is a form of compression that works for any image, but leads to rapid deterioration of image quality when the rate of compression is high. Likewise, reducing the number of yield curve points by relying on interpolation over longer maturity intervals leads to rapid deterioration of curve representation accuracy. Autoencoders (AE) are machine learning algorithms that provide a fundamentally different type of compression. The rate of compression they can achieve for images while maintaining high resolution is orders of magnitude better compared to the most advanced non-AE algorithms such as JPEG. The key to superior performance of AE is that they are optimized for a specific dataset, such as a library of human face images, while general purpose algorithms such as JPEG can compress any image but not nearly as effectively.

As a result of aggressively eliminating any combinations of pixels that do not look like a face from the compressed image representation, something quite remarkable happens – a reverse transformation becomes possible. For traditional image compression algorithms

such as JPEG, uncompressing a random sequence of bits will produce a meaningless image. However, decoding a random point in the low dimensional space of AE latent variables produces an image that represents a realistic looking face. Furthermore, a gradual change in latent space leads to realistic and gradual changes to the image, such as adding a smile.

Sokol [3] proposed leveraging these remarkable properties of AE for finding the optimal set of state variables to represent the yield curve for the purposes of P- and Q-measure model construction. He demonstrated that training AE on historical curve shapes leads to a higher degree of compression than can be achieved using parametric curve representations such as Nelson-Siegel, or classic optimization methods such as PCA. In [4], Andreasen proposed an AE construction method specifically designed for dynamic arbitrage-free models in Q-measure.

The reason AE approach works well for curve compression is that historical curves represent a small fraction of all possible curve shapes, just like human face images represent a small fraction of all possible images. By training on a dataset of historical curves, the AE algorithm finds the most accurate way to represent them using a small number of latent variables.

To obtain sufficient data for such training, Sokol [3] proposed combining curve data from multiple currencies into a single training dataset, something not usually done when calibrating interest rate models. Similar to how training AE on a well-diversified library of face images enhances rather than diminishes its ability to accurately represent individual features of a specific human face, using data from multiple currencies for AE training enhances its ability to accurately represent the curves for each specific currency.

While AE algorithms such as those used by Sokol and Andreasen usually rely on neural networks, we will use the term AE generically throughout the paper to refer to compression algorithms optimized for a specific dataset, whether or not neural networks are used for AE construction. Classical optimization techniques can provide a practical alternative when the use of machine learning for interest rate modeling is not permitted by the bank's policies.

3 Curve Parameterization

Most forward rate models in Q-measure are specified using forward rates for the maturity times T that remain fixed as the observation time t advances. In contrast, historically estimated curve representations such as the Nelson-Siegel formula are specified using time to maturity $\tau = T - t$ defined relative to the observation time t because the absolute maturity time T is meaningless in such context. Because our approach is also based on historical estimation, we will use τ -parameterized variables in forward rate model construction, an approach proposed by Musiela [5] and recently further developed by Lyashenko and Goncharov [6, 7].

The instantaneous forward rate $f(t, \tau)$ observed at time t for time to maturity τ is given by:

$$f(t, \tau) = -\frac{\partial \ln P(t, \tau)}{\partial \tau} \quad (1)$$

where $P(t, \tau)$ is the price of a zero bond with maturity time $t + \tau$ observed at time t .

Let $\hat{f}_Z(\tau, \mathbf{Z})$ be the AE representation for the instantaneous forward rate that depends on time to maturity τ and the latent variable vector $\mathbf{Z} = (Z_1, \dots, Z_K)^T$ where K is the dimension of latent space. Here and throughout the paper the hat symbol will be used to specify low dimensional representations for the corresponding quantities without the hat, in this case $f(t, \tau)$. The forward rate in our model has the following form:

$$f(t, \tau) = \hat{f}_Z(\tau, \mathbf{Z}(t)) + \phi(\tau + t) + O(\sigma^2 t) \quad (2)$$

where $\mathbf{Z}(t)$ is the stochastic process of latent variables, $\phi(T)$ is the deviation of the initial curve at $t = 0$ from the autoencoder representation for maturity T , and the last term is convexity correction which we will examine in detail in what follows. If the initial curve is located in close vicinity of the autoencoder representation $\hat{f}_Z(\tau, \mathbf{Z})$ like most historically observed curves, $\phi(T)$ will be small compared to the level of the modeled rates.

Following the terminology introduced in Bjork and Christensen [8], we will call the forward rate curve family $\hat{f}_Z(\tau, \mathbf{Z})$ the autoencoder (AE) manifold \mathcal{M}_Z^f in the linear space of all forward curves parameterized by $\mathbf{Z} \in \mathbb{R}^K$:

$$\mathcal{M}_Z^f = \left\{ \hat{f}_Z(\tau, \mathbf{Z}) \mid \mathbf{Z} \in \mathbb{R}^K \right\} \quad (3)$$

Here and throughout the paper we use the notation \mathcal{M}_B^A to describe a manifold for A parameterized by B .

4 Time Shift Invariance and Static Arbitrage

A model is said to be static arbitrage-free if it is free of arbitrage for zero volatility. While in theory a model can be dynamic arbitrage-free (i.e., free from arbitrage at the calibrated volatility level) but not static arbitrage-free, practical value of a model that does not work in the simplest case of zero volatility is very questionable. All classical interest rate models in Q-measure are free of static arbitrage by construction. Since this is generally not the case for the forward rate evolution given by (2), we will impose the requirement that our model is free of static arbitrage.

The requirement of no static arbitrage imposes a time shift invariance constraint on a curve representation parameterized by time to maturity τ . Recall that for arbitrage-free evolution with zero volatility, the forward rate for a given absolute maturity time T should be constant. Since $\tau = T - t$, we can write this property using our τ -based parameterization of $f(t, \tau)$ as follows:

$$f(t, T - t) = f(t, T - t)|_{t=0} = f(0, T) \quad (4)$$

Replacing $T - t$ by τ we get:

$$f(t, \tau) = f(0, \tau + t) \quad (5)$$

Substituting (2) into (5), we obtain the following static no-arbitrage constraint on AE curve representations: for every initial latent variable vector \mathbf{Z} and time shift t , there must exist such latent variable vector \mathbf{Z}' that

$$\hat{f}_Z(\tau + t, \mathbf{Z}) = \hat{f}_Z(\tau, \mathbf{Z}') \quad (6)$$

i.e., the curve representation must be invariant to a time shift (more precisely, a shift in τ). In what follows, we will use the terms “static no-arbitrage constraint” and “time shift invariance” interchangeably.

Equation (6) states that for any forward curve that lies on the AE manifold, a curve obtained by removing the initial segment with time to maturity $0 < \tau < t$ and then shifting the rest of the curve back to origin must also lie on the same AE manifold. The objective of AE training is to find the optimal fit to the historical data that satisfies this constraint.

5 Stationarity of the Long Forward Rate

Let $f_\infty(t)$ be the limit value of the instantaneous forward rate $f(t, \tau)$ observed at time t for $\tau \rightarrow \infty$. We assume this limit exists and is finite, consistent with the typical assumptions used in economic theory. A well-known theorem by Dybvig, Ingersoll and Ross [9] states that in a frictionless no-arbitrage economy $f_\infty(t)$ can never fall, i.e., once it reaches a certain level for the observation time t , any lower level at a later time $t' > t$ will result in arbitrage:

$$f_\infty(t') \geq f_\infty(t) \quad \text{if } t' > t \quad (7)$$

They also pointed out that if we make a further assumption that the economy is stationary over the long run, these rates also cannot rise as they would then be unable to come down to their prior levels, and must therefore remain constant.

If the Dybvig, Ingersoll and Ross theorem seems puzzling, we offer the following simple way to understand its meaning on a conceptual level without relying on their ingenious yet difficult to follow original proof. Consider an interest rate shock to the instantaneous forward curve in a stationary economy that occurred a long time ago. The theorem states that the consequences of this shock will eventually decay and will not be felt after an infinite amount of time passes. In a model where interest rates follow a mean-reverting stochastic process, this is equivalent to the requirement that all mean reversion speed parameters must be strictly positive.

Using strictly positive mean reversion speed parameters is a well-understood and widely accepted requirement in Q-measure modelling. We will adopt this requirement for our model, where it takes the form of the following constraint on the autoencoder representation $\hat{f}_Z(\tau, \mathbf{Z})$ for any \mathbf{Z} :

$$\lim_{\tau \rightarrow \infty} \hat{f}_Z(\tau, \mathbf{Z}) = f_\infty \quad (8)$$

where the long rate f_∞ is a constant model parameter that does not depend on the observation time t . Dybvig, Ingersoll and Ross provided rigorous justification for imposing this constraint based on formal no-arbitrage arguments, stating in their paper: “Therefore, it is not permissible, for example, to specify a term structure model with a stochastic factor which is the long (asymptotic) end of the zero-coupon yield curve (unless this factor can only increase over time). In a similar fashion, empirical fittings of yield curves, using, for example, splines, may wish to constrain the asymptote to be constant (or nondecreasing).”

The long rate f_∞ cannot be observed in the market directly and must be estimated by a statistical method. In [10], Sokol proposed estimating f_∞ as the level where regressions of rates with different maturities near the long end of the curve intersect. The level

of f_∞ obtained using this method is broadly in line with the estimate we obtained by optimizing the fit of historical data to the AE manifold. We also found that model results are not overly sensitive to the precise choice of f_∞ , as long as this level remains constant under the model's stochastic process.

6 Arbitrage-Free Interpolation

The AE training methods proposed by Sokol [3] and Andreasen [4] produce low dimensional representation for a finite set of swap rates with discrete maturities. While having the advantage of dealing with market observables directly, the rates produced by AE must then be used as an input to a curve builder to obtain the instantaneous forward rate as a continuous function of τ . In this paper, we will instead build AE for such continuous representation directly. Making AE output the entire interpolated curve rather than term rates for a discrete set of maturities is important for our purposes because our methodology relies on an intricate set of no-arbitrage constraints that would be destroyed by applying bootstrapping after the fact.

We begin from the classic forward curve factor representation with the stationary long rate f_∞ :

$$\hat{f}_X(\tau, \mathbf{X}) = f_\infty + \mathbf{B}(\tau)\mathbf{X} \quad (9)$$

where $\mathbf{X} = (X_1, \dots, X_N)^T$ is a column vector of state variables (factors) and $\mathbf{B}(\tau) = (B_1(\tau), \dots, B_N(\tau))$ is the row vector of basis functions (loadings of these factors). If N is the same as the number of curve builder inputs, (9) will reproduce every curve builder input exactly. If N is less than the number of curve builder inputs, (9) will perform an approximate fit instead. Following the standard approach in Q-measure model construction, in the latter case we will absorb the error in fitting the initial market-implied forward curve into the correction term $\phi(\tau + t)$ in (2) to keep our model strictly arbitrage-free.

In [6, 7], Lyashenko and Goncharov showed that for the forward curve (9) to satisfy the static no-arbitrage condition (6) the basis vector $\mathbf{B}(\tau)$ should be of the form:

$$\mathbf{B}(\tau) = \mathbf{B}_0 \exp(-\tau \mathbf{D}) \quad (10)$$

where \mathbf{D} is a square (generating) matrix and \mathbf{B}_0 is a row vector. The corresponding forward rate representation (9) can be written in the form

$$\hat{f}_X(\tau, \mathbf{X}) = f_\infty + \sum_{i=1}^L \sum_{j=1}^{m(i)} X_{s(i)+j} \tau^{j-1} e^{-\lambda_i \tau} \quad (11)$$

where $\lambda_1, \dots, \lambda_L$ are (distinct) eigenvalues of the generating matrix \mathbf{D} , $m(1), \dots, m(L)$ are their (algebraic) multiplicities¹, and the multiplicity counting function $s(i)$ is defined as follows

$$s(i) = \sum_{j=1}^{i-1} m(j), \quad i = 1, \dots, L \quad (12)$$

¹Geometric multiplicities should be equal to 1 to ensure that the basis functions are linearly independent.

where we use the convention of empty sum being equal to zero. Note that the power terms τ^{j-1} appear in (11) only in the case of non-diagonalizable matrix \mathbf{D} , where some of the multiplicities $m(i)$ are larger than 1.

The Nelson-Siegel [11] basis and its extensions have been the de-facto standard in fitting yield curve shapes for over three decades. The canonical Nelson-Siegel formula has the following form for the instantaneous forward rate:

$$\hat{f}_X^{\text{NS}}(\tau, \mathbf{X}) = X_0 + X_1 e^{-\lambda\tau} + X_2 \lambda \tau e^{-\lambda\tau}. \quad (13)$$

This representation is static arbitrage-free (i.e., invariant to time shift) as its basis

$$\mathbf{B}(\tau) = (1, e^{-\lambda\tau}, \tau e^{-\lambda\tau}) \quad (14)$$

can be written in the form (10) with non-diagonalizable generating matrix

$$\mathbf{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \lambda & -1 \\ 0 & 0 & \lambda \end{pmatrix} \quad (15)$$

However, the Nelson-Siegel representation (13) is not a special case of our form (9) because it allows the maturity-independent term X_0 to vary from one curve observation to the next, while in our form (9) $f_\infty = X_0$ is stationary (i.e., does not change under the action of the model's stochastic process). Because all representations of the Nelson-Siegel family share the property of allowing X_0 and therefore the long forward rate f_∞ to vary, they are incompatible with the Dybvig-Ingersoll-Ross theorem or the requirement that all mean reversion speed parameters are strictly positive, and we will not consider them further in this paper.

With the notable exception of the Nelson-Siegel basis and its extensions, quantitative finance models typically use pure exponential bases where the generating matrix \mathbf{D} is diagonalizable and the forward rate representation (11) takes an especially simple form:

$$\hat{f}_X(\tau, \mathbf{X}) = f_\infty + \sum_{n=1}^N X_n e^{-\lambda_n \tau} \quad (16)$$

In the rest of the paper, we assume all the eigenvalues λ_i of the generating matrix \mathbf{D} to be strictly positive in order to satisfy the constant long rate requirement (8).

7 Forward Rate Manifold

Using the forward curve representation (9), we can build the forward rate curve manifold \mathcal{M}_Z^f by first building an \mathbf{X} -manifold (i.e., a manifold for \mathbf{X}):

$$\mathcal{M}_Z^X = \{\mathbf{X} = \mathbb{X}(\mathbf{Z}) \mid \mathbf{Z} \in \mathbb{R}^K\} \quad (17)$$

with the AE transformation $\mathbb{X} : \mathbb{R}^K \rightarrow \mathbb{R}^N$ trained to the historical observations of factor vectors \mathbf{X} obtained by bootstrapping historical rate data using representation (9), and then setting

$$\mathcal{M}_Z^f = \left\{ \hat{f}_Z(\tau, \mathbf{Z}) = f_\infty + \mathbf{B}(\tau) \mathbb{X}(\mathbf{Z}) \mid \mathbf{Z} \in \mathbb{R}^K \right\} \quad (18)$$

Note that the K -dimensional f -manifold \mathcal{M}_Z^f is embedded in the full N -dimensional linear (affine) manifold (space) of forward rate curves

$$\mathcal{M}_X^f = \left\{ \hat{f}_X(\tau, \mathbf{X}) = f_\infty + \mathbf{B}(\tau)\mathbf{X} \mid \mathbf{X} \in \mathbb{R}^N \right\} \quad (19)$$

While the full linear (affine) manifold \mathcal{M}_X^f satisfies the static no-arbitrage property (6) because of (10), the (nonlinear) manifold \mathcal{M}_Z^f generally does not.

It is easy to see that, because of the property (10), the (nonlinear) f -manifold \mathcal{M}_Z^f satisfies the static no-arbitrage property (6) if and only if the corresponding X-manifold \mathcal{M}_Z^X defined by (17) is invariant with respect to multiplication by $e^{-t\mathbf{D}}$ for any $t > 0$ in the sense that if $\mathbf{X} \in \mathcal{M}_Z^X$ then $e^{-t\mathbf{D}}\mathbf{X} \in \mathcal{M}_Z^X$. We use the following notation for this invariance property

$$e^{-t\mathbf{D}}\mathcal{M}_Z^X \equiv \mathcal{M}_Z^X, \quad t > 0 \quad (20)$$

Due to our assumption of all eigenvalues of the generating matrix \mathbf{D} being positive, the invariance condition (20) implies that the zero point should belong to the manifold \mathcal{M}_Z^X , at least asymptotically.

8 Linear Manifold Construction

The case of AE where all activation functions are linear is very instrumental since it is equivalent to the PCA (principal component analysis) representation. This is a very important benchmark case because the PCA approach is widely used in financial analysis and modeling. In this case, the X-manifold defining transformation $\mathbb{X} : \mathbb{R}^K \rightarrow \mathbb{R}^N$ has the affine representation

$$\mathbb{X}(\mathbf{Z}) = \mathbf{X}_0 + \mathbf{G}\mathbf{Z} \quad (21)$$

where \mathbf{X}_0 is a constant N -dimensional (column) vector and \mathbf{G} is an $N \times K$ matrix of full rank.

Typically, the PCA approach is applied to increments (returns) rather than levels and is linear rather than affine. However, when applied to levels rather than increments, the linear PCA representation must be affine with the intercept vector \mathbf{X}_0 .

In this section, we examine when the X-manifold \mathcal{M}_Z^X satisfies the static no-arbitrage invariance condition (20) in the linear (PCA) case. We want to see when the PCA transformation (21) preserves the static no-arbitrage property of the full forward rate manifold \mathcal{M}_X^f .

First, we note that for the X-manifold \mathcal{M}_Z^X to (asymptotically) contain the zero point as pointed out in the previous section, the N -dimensional hyper-plane defined by (21) should contain zero. This means that there exists \mathbf{Z}_0 such that $\mathbf{G}\mathbf{Z}_0 = -\mathbf{X}_0$ and thus (21) can be written as

$$\mathbb{X}(\mathbf{Z}) = \mathbf{G}(\mathbf{Z} - \mathbf{Z}_0) \quad (22)$$

Therefore by changing variables from \mathbf{Z} to $\mathbf{Z} - \mathbf{Z}_0$ we can write (21) in the linear form

$$\mathbb{X}(\mathbf{Z}) = \mathbf{G}\mathbf{Z} \quad (23)$$

where we kept the same latent vector notation \mathbf{Z} for simplicity. Thus the X-manifold

$$\mathcal{M}_Z^X = \{\mathbf{X} = \mathbf{G}\mathbf{Z} \mid \mathbf{Z} \in \mathbb{R}^K\} \quad (24)$$

is a K -dimensional linear subspace (hyper-plane) in the N -dimensional linear space of state vectors \mathbf{X} .

We first consider the case of diagonalizable generating matrix \mathbf{D} , where the full forward rate manifold \mathcal{M}_X^f can be written as

$$\mathcal{M}_X^f = \left\{ \hat{f}_X(\tau, \mathbf{X}) = f_\infty + \sum_{n=1}^N X_n e^{-\tau \lambda_n} \right\} \quad (25)$$

with λ_i being the distinct eigenvalues² of matrix \mathbf{D} .

In Appendix A.1 we prove that for the X-manifold \mathcal{M}_Z^X given by (24) to satisfy the static no-arbitrage invariance condition (20), there should be K eigenvectors $\mathbf{e}_{i_1}, \dots, \mathbf{e}_{i_K}$ of matrix \mathbf{D} that span the linear subspace \mathcal{M}_Z^X and that the forward rate manifold \mathcal{M}_Z^f can be written as follows

$$\mathcal{M}_Z^f = \left\{ \hat{f}_Z(\tau, \mathbf{Z}) = f_\infty + \sum_{k=1}^K Z_k e^{-\tau \lambda_{i_k}} \right\} \quad (26)$$

Compare this to the full forward rate manifold \mathcal{M}_X^f given by (25).

Thus, we have the following important result: *In the case when matrix \mathbf{D} is diagonalizable, i.e., all eigenvalues have (algebraic) multiplicity of one, the only dimensionality reduction that preserves the static no-arbitrage property (20) is dropping some of the eigenvalues of the generating matrix \mathbf{D} .*

In the general case of the generating matrix \mathbf{D} with eigenvalue multiplicities that can be larger than 1, we get a more general result that *the only linear dimensionality reductions that preserve the static no-arbitrage invariance property (20) consist of reducing multiplicities of some of the eigenvalues of the generating matrix \mathbf{D} , which includes dropping some eigenvalues by reducing their multiplicities to zero.* The proof can be found in Appendix A.2.

This result is very instructive. In particular, it shows that an empirically estimated principal component basis would not generally be suitable for no-arbitrage modeling of a yield curve as it is unlikely to satisfy the static no-arbitrage condition. This may explain why previous attempts to construct PCA-based risk-neutral term structure models (see, for instance, Rebonato [12]) encountered formidable challenges.

This result also indicates that the appropriate course of action for finding the optimal linear representation is not starting from (9) with large N and then reducing dimension using a linear transformation such as PCA, but instead starting from small N and finding the set of λ_n that provide the best fit to the historical data. Otherwise, there is no guarantee that parameters λ_n optimized for the high dimension will have a subset that is optimal for the low dimension. As an added benefit, starting from lower dimension makes it possible to include historical data that has missing maturity points.

²Eigenvalues of the generating matrix should be distinct for the basis to be composed of linearly independent functions.

9 Nonlinear Manifold Construction

Recall that a static arbitrage-free f -manifold must be invariant to the time shift. This means the \mathbf{X} -manifold $\mathcal{M}_Z^X = \{\mathbf{X} = \mathbb{X}(\mathbf{Z}) \mid \mathbf{Z} \in \mathbb{R}^K\}$ must be invariant with respect to multiplication by the exponential matrix $e^{-t\mathbf{D}}$ for any $t > 0$ as per (20). If we train the $\mathbb{X}(\mathbf{Z})$ autoencoder to the historical data directly, the resulting manifold \mathcal{M}_Z^X will not automatically satisfy the static no-arbitrage condition. However, if we instead start from a generating manifold with one less dimension $(Y_1, \dots, Y_{K-1}) \in \mathbb{R}^{K-1}$:

$$\mathcal{M}_Y^X = \{\mathbf{X} = \mathbb{X}(\mathbf{Y}) \mid \mathbf{Y} \in \mathbb{R}^{K-1}\} \quad (27)$$

and define the full K -dimensional manifold $\mathcal{M}_{t,Y}^X$ as the result of applying the time shift to this generating manifold:

$$\mathcal{M}_{t,Y}^X = \{\mathbf{X} = e^{-t\mathbf{D}}\mathbb{X}(\mathbf{Y}) \mid t \in \mathbb{R}, \mathbf{Y} \in \mathbb{R}^{K-1}\} \quad (28)$$

the static no-arbitrage condition (20) will be satisfied by construction. Training AE with $K - 1$ latent variables \mathbf{Y} instead of K latent variables \mathbf{Z} to the historical data is a practical and effective way to perform optimization constrained by the static no-arbitrage invariance condition (20).

The nontrivial geometry of the generating manifold is visualized in Figures 1, 2 and 3. For $K = 2$, the generating manifold \mathcal{M}_Y^X is a ring encircling the origin $\mathbf{X} = 0$ and the generated manifold \mathcal{M}_Z^X is a two-dimensional surface whose edge is the generating manifold ring (Figure 2). For $K = 3$, the generating manifold \mathcal{M}_Y^X is the surface of a sphere encircling the origin and the generated manifold \mathcal{M}_Z^X is the internal volume of this sphere (Figure 3). While only the first three dimensions of \mathbf{X} can be visualized, the actual dimension of \mathbf{X} may be greater than $N = 3$.

The latent variables \mathbf{Y} of the generating manifold \mathcal{M}_Y^X span all possible zero-volatility trajectories by which \mathbf{X} may evolve with the passage of time while $Z_0 = t$ is responsible for the motion along these trajectories toward the origin as shown in Figure 4. As each trajectory approaches the origin, all forward rates converge to the equilibrium level f_∞ as $t \rightarrow \infty$.

Its ability of the generating manifold ring to deviate from the PCA plane for $K = 2$ and from the PCA hypersurface for $K > 2$ is the source of the greater capacity for optimization offered by the nonlinear AE-based manifolds compared to the linear ones.

As the time shift variable $t = Z_0$ is responsible for the distance to the origin $\mathbf{X} = 0$ it is natural to use polar coordinates for all remaining latent variables \mathbf{Y} . For $K = 2$, we can choose the sole latent variable Y_1 to be the longitude within the generating manifold ring and for $K = 3$ we can choose $Y_{1,2}$ to be the longitude and latitude within the generating manifold sphere.

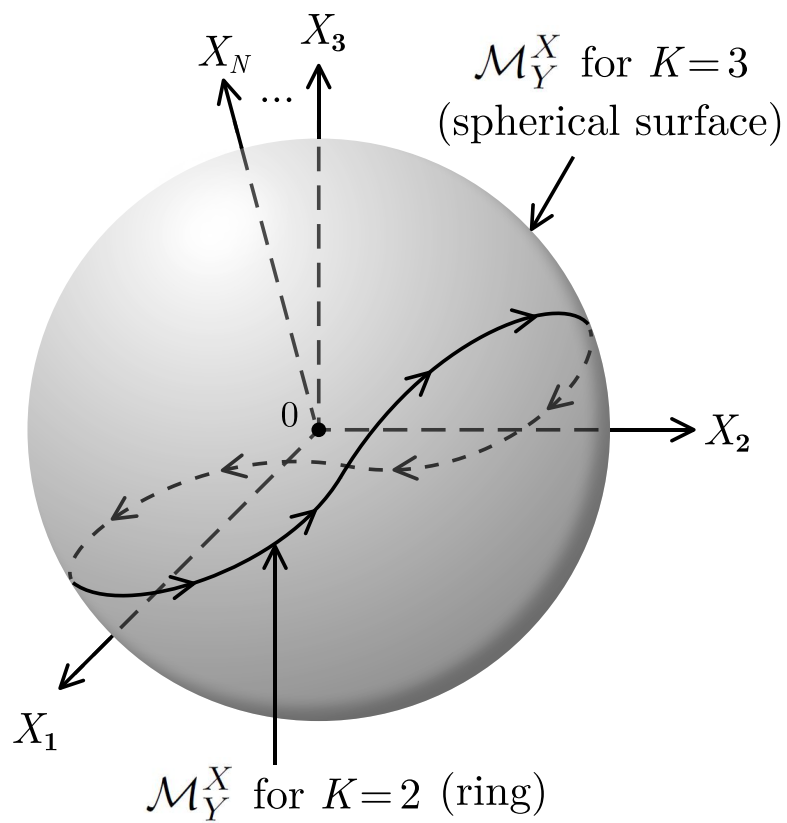


Figure 1: The generating manifold \mathcal{M}_Y^X is a ring for $K = 2$ and is a spherical surface for $K = 3$.

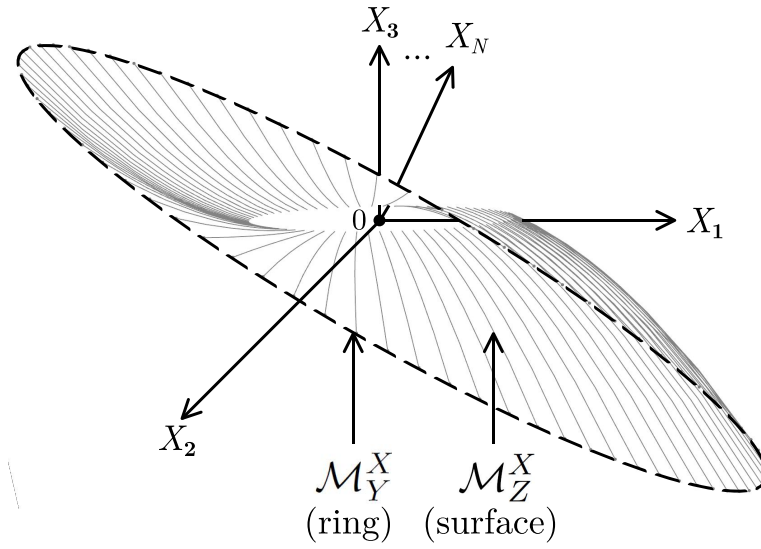


Figure 2: For $K = 2$, the generating manifold \mathcal{M}_Y^X is a ring (shown as a dashed line) and the generated manifold \mathcal{M}_Z^X is a surface (shown as solid lines).

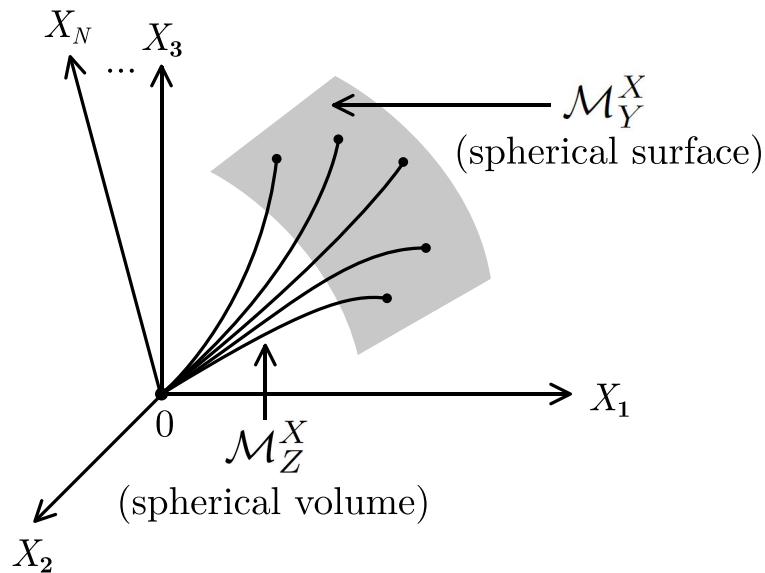


Figure 3: For $K = 3$, the generating manifold \mathcal{M}_Y^X is the surface of a sphere (a segment is shown) and the generated manifold \mathcal{M}_Z^X is the inner volume of this sphere.

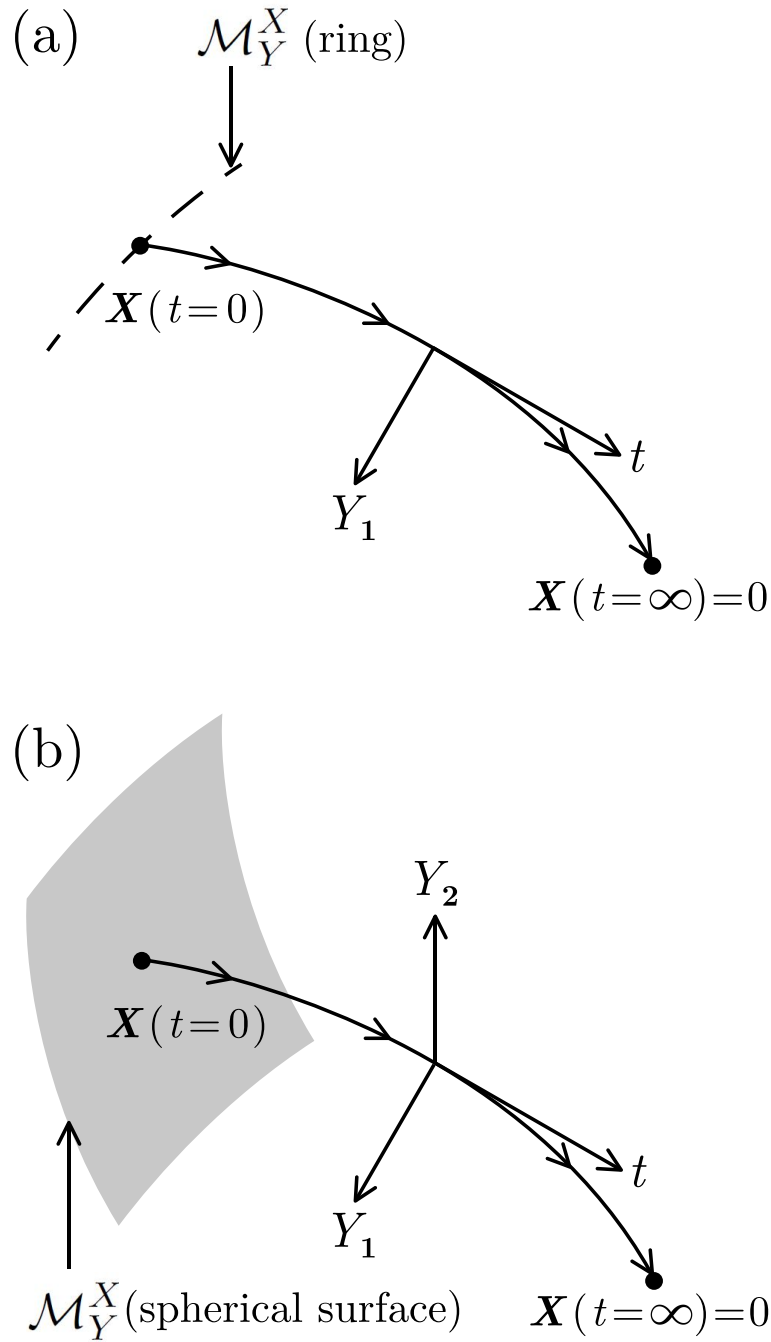


Figure 4: Panel (a), $K = 2$. Panel (b), $K = 3$. Each arbitrage free zero-volatility trajectory (solid lines) originates at a single point \mathbf{Y} of the generating manifold \mathcal{M}_Y^X evolves toward the origin $\mathbf{X} = 0$ with the passage of time t . The latent variables \mathbf{Y} of the generating manifold traverse the trajectories (while not necessarily being orthogonal to them) while $Z_0 = t$ is tangential to the trajectories. The origin $\mathbf{X} = 0$ corresponds to the flat curve where all forward rates are equal to f_∞ .

10 Risk-Neutral Model

In this section, we derive general conditions for the forward rate manifold \mathcal{M}_Z^f defined by (18) to admit no-arbitrage forward curve evolution. We will assume that the AE mapping $\mathbb{X}(\mathbf{Z})$ is smooth (twice continuously differentiable), which can be ensured by selecting smooth activation functions.

We will say that the forward rate manifold \mathcal{M}_Z^f is dynamic arbitrage-free if for any $\mathbf{Z}_0 \in \mathbb{R}^K$ there exists a process $\mathbf{Z}(t)$ defined by

$$d\mathbf{Z}(t) = \boldsymbol{\mu}^Z(t)dt + \boldsymbol{\sigma}^Z(t)d\mathbf{W}(t), \quad \mathbf{Z}(0) = \mathbf{Z}_0 \quad (29)$$

such that the manifold \mathcal{M}_Z^f bound forward curve evolution given by

$$f(t, \tau) := \hat{f}_Z(\tau, \mathbf{Z}(t)) = f_\infty + \mathbf{B}(\tau)\mathbb{X}(\mathbf{Z}(t)) \quad (30)$$

is arbitrage-free.³ In equation (29), $\boldsymbol{\mu}^Z(t)$ is an adapted vector of size K , $\boldsymbol{\sigma}^Z(t)$ an adapted volatility matrix of size $K \times M$, and $\mathbf{W}(t)$ a standard M -dimensional Q-Brownian motion, where $M \leq K$.

The dynamic no-arbitrage condition for the instantaneous forward rate $f(t, \tau)$ is given by the Musiela [5] parameterization of the Heath-Jarrow-Morton (HJM) [13] equation

$$df(t, \tau) = \left(\frac{\partial f(t, \tau)}{\partial \tau} + \boldsymbol{\sigma}^f(t, \tau)^T \int_0^\tau \boldsymbol{\sigma}^f(t, u) du \right) dt + \boldsymbol{\sigma}^f(t, \tau)^T d\mathbf{W}(t) \quad (31)$$

where $\boldsymbol{\sigma}^f(t, \tau)$ is the adapted column volatility vector of the forward. The first drift term simply captures the effect of advancing observation time t on the forward rate parameterized as a function of $\tau = T - t$. It appears only as a result of the changing frame of reference, and is absent when the HJM model is written down in its canonical form for the absolute maturity time T rather than $\tau = T - t$.

The latent vector process $\mathbf{Z}(t)$ defines the manifold \mathcal{M}_Z^X bound X-process

$$\mathbf{X}(t) = \mathbb{X}(\mathbf{Z}(t)) \quad (32)$$

that satisfies the following SDE:

$$d\mathbf{X}(t) = \left(\frac{\partial \mathbb{X}(\mathbf{Z}(t))}{\partial \mathbf{Z}} \boldsymbol{\mu}^Z(t) + \boldsymbol{\Phi}(t) \right) dt + \frac{\partial \mathbb{X}(\mathbf{Z}(t))}{\partial \mathbf{Z}} \boldsymbol{\sigma}^Z(t) d\mathbf{W}(t) \quad (33)$$

where $\boldsymbol{\Phi}(t)$ is the convexity term:

$$\boldsymbol{\Phi}(t) = \frac{1}{2} \sum_{i,j=1}^K \frac{\partial^2 \mathbb{X}(\mathbf{Z}(t))}{\partial Z_i \partial Z_j} [\mathbf{v}^Z(t)]_{i,j} \quad (34)$$

and $\mathbf{v}^Z(t)$ is the variance matrix of \mathbf{Z} :

$$\mathbf{v}^Z(t) = \boldsymbol{\sigma}^Z(t) (\boldsymbol{\sigma}^Z(t))^T \quad (35)$$

³Following Bjork and Christensen (1999), we can require instead a local no-arbitrage property that is limited to an open set of initial values \mathbf{Z}_0 and time interval $[0, \epsilon)$.

Plugging the forward rate representation (30) into the Musiela HJM equation (31) and using (10) and (33) we get, dropping dependence on t for readability,

$$\sigma^f(\tau) = B(\tau) \frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \sigma^Z \quad (36)$$

and

$$B(\tau) \left(\frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \mu^Z + \Phi \right) = -B(\tau) D\mathbb{X}(\mathbf{Z}) + B(\tau) v^X \int_0^\tau B(s)^T ds \quad (37)$$

where v^X is the variance matrix of \mathbf{X} :

$$v^X = \frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} v^Z \left(\frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \right)^T \quad (38)$$

In [6, 7], Lyashenko and Goncharov showed that the last term in equation (37) can be written in the form

$$B(\tau) v^X \int_0^\tau B(s)^T ds = \tilde{B}(\tau) \Omega \quad (39)$$

where $\tilde{B}(\tau)$ is a basis of the form (10) that includes (extends) basis $B(\tau)$ and vector Ω has entries that are linear combinations of entries of matrix v^X .

Thus, for the manifold \mathcal{M}_Z^f bound forward curve evolution given by (30) to be arbitrage free, the drift μ^Z of the latent vector process $\mathbf{Z}(t)$ defined by (29) should satisfy the following condition:

$$B(\tau) \frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \mu^Z = -B(\tau) D\mathbb{X}(\mathbf{Z}) - B(\tau) \Phi + \tilde{B}(\tau) \Omega \quad (40)$$

The dynamic no-arbitrage condition (40) represents a constraint on the mapping $\mathbb{X}(\mathbf{Z})$ since it generally cannot be solved for μ^Z because the dimensionality of μ^Z is K while the dimensionality of the space spanned by the basis $B(\tau)$ is $N > K$ and the dimensionality of the extended basis $\tilde{B}(\tau)$ is greater than N .

The term $B(\tau)\Phi$ is a convexity adjustment that is zero in the linear case while the term $\tilde{B}(\tau)\Omega$ is the HJM arbitrage adjustment term. The vectors Φ and Ω are linear with respect to the entries of the variance matrix v^Z and thus are quadratic with respect to the entries of the volatility vector σ^Z .

In the zero volatility case $\sigma^Z = 0$, the dynamic no-arbitrage condition (40) becomes:

$$\frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \mu^Z = -D\mathbb{X}(\mathbf{Z}) \quad (41)$$

Reintroducing back the time dependence, we note that in the zero volatility case the condition above is equivalent to

$$d\mathbb{X}(\mathbf{Z}(t)) = -D\mathbb{X}(\mathbf{Z}(t))dt \quad (42)$$

which implies

$$\mathbb{X}(\mathbf{Z}(t)) = e^{-tD} \mathbb{X}(\mathbf{Z}_0) \quad (43)$$

We can immediately see that condition (43) is equivalent to the static no-arbitrage condition (20). It means that we can always solve (41) for μ^Z if the \mathbf{X} -manifold \mathcal{M}_Z^X

satisfies the invariance condition (20). Thus, we have obtained the following important result: *the general dynamic no-arbitrage condition (40) is satisfied to the approximation order of $O(\sigma^2 t)$ if the static no-arbitrage condition (20) holds.*

It is interesting to note that the zero-volatility condition (41) has geometric interpretation of vector $\mathbf{D}\mathbb{X}(\mathbf{Z})$ being tangential to the manifold \mathcal{M}_Z^X at the point $\mathbb{X}(\mathbf{Z})$. Since the initial point \mathbf{Z}_0 can be anything, this implies that for the manifold \mathcal{M}_Z^X to satisfy the static no-arbitrage condition (20), for any $\mathbf{X} \in \mathcal{M}_Z^X$ the vector $\mathbf{D}\mathbf{X}$ should be tangential to \mathcal{M}_Z^X at the point \mathbf{X} . The dynamic no-arbitrage condition (40) also has a geometric interpretation. Indeed, it is equivalent to its right hand side being tangential to the forward rate manifold \mathcal{M}_Z^f . This is fully consistent with the results of Björk and Christensen [8].

In the linear case, the convexity term $\mathbf{B}(\tau)\Phi$ drops out and the dynamic no-arbitrage condition (40) becomes

$$\mathbf{B}(\tau) \frac{\partial \mathbb{X}(\mathbf{Z})}{\partial \mathbf{Z}} \boldsymbol{\mu}^Z = -\mathbf{B}(\tau) \mathbf{D}\mathbb{X}(\mathbf{Z}) + \tilde{\mathbf{B}}(\tau) \boldsymbol{\Omega} \quad (44)$$

The linear case was considered in full generality by Lyashenko and Goncharov in [6, 7]. They showed that a linear manifold \mathcal{M}_Z^f admits dynamic no-arbitrage evolution for any (reasonable) volatility process $\boldsymbol{\sigma}^Z(t)$ if extended to the linear space spanned by the larger basis $\tilde{\mathbf{B}}$. Therefore, in the linear case we can construct such linear manifold spanned by a finite basis of functions as long as the basis is appropriately chosen.

A very interesting and insightful observation is that by using the latent variables of the generating manifold \mathcal{M}_Y^X given by (27), we have the term $-\mathbf{B}(\tau) \mathbf{D}\mathbb{X}(\mathbf{Z})$ drop from the dynamic no-arbitrage equation (37), which effectively converts the Musiela τ -parameterization of the HJM equation to its canonical T -parameterized form under the forward rate representation (9).

11 Linear Manifolds and Short Rate Models

Consider an N -factor Gaussian short rate model of the form:

$$\begin{aligned} r(t) &= \psi(t) + \sum_{n=1}^N X_n(t) \\ dX_n(t) &= -\lambda_n X_n(t) dt + \sigma_n(t) dW_n(t) \end{aligned} \quad (45)$$

where λ_n are constant and positive mean reversion speed parameters each having a distinct value, $\psi(t)$ and $\sigma_n(t)$ are deterministic functions, and $W_1(t), \dots, W_N(t)$ are correlated standard Brownian motions in the risk-neutral measure whose numeraire is the money-market account accruing continuously at the rate $r(t)$. We can set the initial value of each state variable to zero without loss of generality: $X_n(0) = 0$. The function $\psi(t)$ is used to match the initial ($t = 0$) term structure. In the particular case of $N = 2$, model (45) is the two-factor Hull-White model [14] in its additive representation, see Brigo and Mercurio [15].

Under the model specification (45), zero-coupon bond prices at time t with maturity time $t + \tau$ can be expressed in closed form:

$$P(t, \tau) = \exp \left[- \int_t^{t+\tau} \psi(u) du - \sum_{n=1}^N x_n(t) B_n(\tau) + \frac{1}{2} V(t, \tau) \right] \quad (46)$$

where $B_n(\tau) = (1 - e^{-\lambda_n \tau})/\lambda_n$ and $V(t, \tau)$ is a deterministic function of t and τ representing the convexity terms, the analytical expression for which is omitted here for brevity.

The forward rate curve at time t can then be represented as follows:

$$f(t, \tau) = f(0, t + \tau) + \sum_n X_n(t) e^{-\lambda_n \tau} + O(\sigma^2 t) \quad (47)$$

where the last term $O(\sigma^2 t)$ is a convexity correction. Inspecting (47), we immediately recognize representation (2) with the linear manifold form given by (16). We therefore conclude that the Gaussian short rate model (45) belongs to the family of linear manifold models.

Because the linear manifold (47) generated by the model (45) depends only on the model's mean-reversion speed parameters λ_n , but not on its volatilities $\sigma_n(t)$, we can estimate mean reversion from the linear manifold fit to the historical data before calibrating volatility. This approach provides a novel alternative to the standard set of ad-hoc techniques for estimating these parameters in (45) and similar models using a global fit.

12 Conclusion

In this paper, we presented a new type of Q-measure interest rate model constructed from a nonlinear AE-based representation of the yield curve as a function of few state variables that is optimized to represent the historical data with least error. Thanks to the high compression rate of autoencoders, the stochastic process in our model can accurately represent the curve using as few as two or three dimensions, permitting stable and reliable historical estimation. Our approach provides an attractive alternative to the standard way of incorporating historical data into Q-measure models by estimating historical correlation. We also established a connection between the arbitrage-free linear curve representations and Gaussian short rate models that led to a new way of estimating non-calibrated parameters of these models from the historical data.

The benefits of our approach become evident if we consider a hypothetical economy where all historical observations lie on the AE manifold exactly rather than approximately. Because the change of measure only alters the probability of states but cannot create new states, any Q-measure model that can reach a state outside the manifold with non-zero probability will permit arbitrage. Specifically, such model will assign a non-zero price to options that pay only in states away from the manifold. Because the curve moves within the AE manifold only, these payouts will never occur and selling such options will result in riskless profits. A Q-measure model in such hypothetical economy is only arbitrage-free if it generates future states that lie exactly on the AE manifold. It is reasonable to assume that generating curves in the vicinity of AE manifold will remain a beneficial model property even when AE provides an approximate rather than exact fit to the historical data.

The conclusion that properties of scenarios observed in the real-world can be used to constrain Q-measure dynamics may seem surprising at first. Recall however that Q-measure models routinely do the same when two market observables are in a deterministic relationship, such as the relationship between the price of a basket of stocks and its

constituents, or the relationship between two FX rates and their cross-rate. The SABR model [16], whose frequently cited benefit is the ability to capture the historical relationship between the level of underlying and its volatility, provides an example when such historical relationship is statistical rather than deterministic. Our case is very similar in the sense that interest rates of different maturities have historically exhibited a near deterministic nonlinear relationship that can be parameterized using a small number of latent variables.

Bjork and Christensen [8] previously considered the constraints on Q-measure models that arise when future curves lie exactly on the representations produced by the Nelson-Siegel family of curve representations [11, 17]. They found these constraints quite restrictive, making models that respect them exactly impractical for pricing applications.

Our approach recognizes that the curves cannot lie on the AE manifold exactly without introducing a highly restrictive additional set of constraints on volatility that would render the model unsuitable for practical use. By permitting a small convexity-driven $O(\sigma^2 t)$ departure from the manifold to preserve the dynamic no-arbitrage property, we made our model consistent with any form of volatility, including normal, lognormal, or even stochastic, while still accurately reproducing historical yield curve shapes.

References

- [1] F. Black and M. Scholes, “The pricing of options and corporate liabilities,” *Journal of Political Economy*, vol. 81(3), pp. 637–654, 1973.
- [2] R. C. Merton, “Theory of rational option pricing,” *The Bell Journal of Economics and Management Science*, vol. 4(1), pp. 141–183, 1973.
- [3] A. Sokol, “Autoencoder Market Models for Interest Rates.” Working Paper, SSRN <https://ssrn.com/abstract=4300756>, 2022.
- [4] J. Andreasen, “Decoding the Autoencoder,” *Wilmott*, vol. September, 2023.
- [5] M. Musiela, “Stochastic pdes and term structure models,” *Journées Internationales de Finance, IGR-AFFI*, vol. June, 1993.
- [6] A. Lyashenko and Y. Goncharov, “Bridging P-Q Modeling Divide with Factor HJM Modeling Framework.” Working Paper, SSRN <https://www.ssrn.com/abstract=3995533>, 2021.
- [7] A. Lyashenko and Y. Goncharov, “Introducing the Factor Heath-Jarrow-Morton Term Structure Modelling Framework,” *Risk*, June 2023.
- [8] T. Björk and B. Christensen, “Interest rate dynamics and consistent forward rate curves,” *Mathematical Finance*, vol. 9, 1999.
- [9] P. H. Dybvig, J. E. Ingersoll, Jr., and S. A. Ross, “Long Forward and Zero-Coupon Rates Can Never Fall,” *The Journal of Business*, vol. 69, no. 1, p. 1, 1996.
- [10] A. Sokol, *Long-term Portfolio Simulation: For XVA, Limits, Liquidity and Regulatory Capital*. Risk Books, 2014.
- [11] C. R. Nelson and A. F. Siegel, “Parsimonious Modeling of Yield Curves,” *The Journal of Business*, vol. 60, no. 4, p. 473, 1987.
- [12] R. Rebonato, *Bond Pricing and Yield Curve Modeling: A Structural Approach*. Cambridge University Press, 2018.
- [13] D. Heath, R. Jarrow, and A. Morton, “Bond Pricing and the Term Structure of Interest Rates: A New Methodology for Contingent Claims Valuation,” *Econometrica*, vol. 60, no. 1, pp. 77–105, 1992.
- [14] J. C. Hull and A. D. White, “Numerical Procedures for Implementing Term Structure Models II: Two-Factor Models,” *The Journal of Derivatives*, vol. 2, no. 2, pp. 37–48, 1994.
- [15] D. Brigo and F. Mercurio, “On Deterministic Shift Extensions of Short Rate Models.” Working Paper, SSRN <http://www.ssrn.com/abstract=292060>, 2001.
- [16] P. Hagan, D. Kumar, A. Lesniewski, and D. Woodward, “Managing smile risk,” *Wilmott Magazine*, vol. 1, pp. 84–108, 01 2002.
- [17] L. E. Svensson, “Estimating Forward Interest Rates with the Extended Nelson & Siegel Method,” *Sveriges Riksbank Quarterly Review*, vol. 3, no. 1, pp. 13–26, 1995.

A Proof for the Linear Case

In this Appendix, we provide formal proof for the results presented in the linear case where the X-manifold \mathcal{M}_Z^X is given by (24)

$$\mathcal{M}_Z^X = \{\mathbf{X} = \mathbf{G}\mathbf{Z} \mid \mathbf{Z} \in \mathbb{R}^K\} \quad (48)$$

with \mathbf{G} being an $N \times K$ matrix of full rank. Define

$$\mathbf{\Pi} = \mathbf{G}(\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T \quad (49)$$

a $N \times N$ symmetric matrix of rank K that satisfies $\mathbf{\Pi}\mathbf{\Pi} = \mathbf{\Pi}$ and

$$\mathbf{\Pi}\mathbf{X} = \mathbf{X}, \quad \mathbf{X} \in \mathcal{M}_Z^X \quad (50)$$

Thus $\mathbf{\Pi}$ is an orthogonal projection matrix onto the linear subspace \mathcal{M}_Z^X and we have

$$\mathcal{M}_Z^X = \{\mathbf{X} = \mathbf{\Pi}\mathbf{Y} \mid \mathbf{Y} \in \mathbb{R}^N\} \quad (51)$$

Therefore the invariance property (20) can be written in the form

$$(\mathbf{\Pi} - \mathbf{I})e^{-t\mathbf{D}}\mathbf{\Pi}\mathbf{Y} = 0, \quad \mathbf{Y} \in \mathbb{R}^N, t \geq 0 \quad (52)$$

where \mathbf{I} is the N -dimensional unit matrix.

A.1 Diagonalizable Generating Matrix

We first consider the case of diagonalizable generating matrix \mathbf{D} , where we have

$$e^{-t\mathbf{D}} = \sum_{i=1}^N e^{-t\lambda_i} \mathbf{e}_i \mathbf{e}_i^T \quad (53)$$

with λ_i being the distinct eigenvalues⁴ of matrix \mathbf{D} and \mathbf{e}_i being the corresponding eigenvectors that are normalized to satisfy $\mathbf{e}_i^T \mathbf{e}_j = \delta_{i,j}$, where $\delta_{i,j}$ is the Kronecker delta function. Plugging (53) into (52) we get

$$\sum_{i=1}^N e^{-t\lambda_i} (\mathbf{\Pi} - \mathbf{I}) \mathbf{e}_i \mathbf{e}_i^T \mathbf{\Pi}\mathbf{Y} = 0, \quad \mathbf{Y} \in \mathbb{R}^N, t \geq 0 \quad (54)$$

Since $e^{-t\lambda_i}$, $i = 1, \dots, N$ are linearly independent functions of t , the above equation is equivalent to

$$(\mathbf{\Pi} - \mathbf{I}) \mathbf{e}_i \mathbf{e}_i^T \mathbf{\Pi}\mathbf{Y} = 0, \quad \mathbf{Y} \in \mathbb{R}^N, i = 1, \dots, N \quad (55)$$

Setting $\mathbf{Y} = \mathbf{e}_i$ and multiplying the above equality by \mathbf{e}_i^T from the left, we get the following equality after rearranging terms and using $\mathbf{e}_i^T \mathbf{e}_i = 1$

$$\mathbf{e}_i^T \mathbf{\Pi} \mathbf{e}_i (\mathbf{e}_i^T \mathbf{\Pi} \mathbf{e}_i - 1) = 0, \quad i = 1, \dots, N \quad (56)$$

This equality implies that for any $i = 1, \dots, N$, the scalar $\mathbf{e}_i^T \mathbf{\Pi} \mathbf{e}_i$ is either 0 or 1. Since $\mathbf{\Pi}$ is an orthogonal projection matrix, this means that either $\mathbf{\Pi} \mathbf{e}_i = 0$ or $\mathbf{\Pi} \mathbf{e}_i = \mathbf{e}_i$. Since the eigenvectors $\mathbf{e}_1, \dots, \mathbf{e}_N$ span the whole space \mathbb{R}^N , then there are K eigenvectors

⁴Eigenvalues of the generating matrix should be distinct for the basis to be composed of linearly independent functions.

$\mathbf{e}_{i_1}, \dots, \mathbf{e}_{i_K}$ that span the linear subspace \mathcal{M}_Z^X and the forward rate manifold \mathcal{M}_Z^f can be written in the form

$$\mathcal{M}_Z^f = \left\{ \hat{f}_Z(\tau, \mathbf{Z}) = f_\infty + \sum_{k=1}^K Z_k e^{-\tau \lambda_{i_k}} \right\} \quad (57)$$

Compare this to the full forward rate manifold \mathcal{M}_X^f

$$\mathcal{M}_X^f = \left\{ \hat{f}_X(\tau, \mathbf{X}) = f_\infty + \sum_{n=1}^N X_n e^{-\tau \lambda_n} \right\} \quad (58)$$

A.2 Non-Diagonalizable Generating Matrix

Let us now consider the general case of a possibly non-diagonalizable generating matrix \mathbf{D} , which means that its eigenvalues can have multiplicities greater than 1. Assuming the basis $\mathbf{B}(\tau)$ to be standardized as described in Lyashenko and Goncharov [6, 7], the generating matrix \mathbf{D} can be written in the following block-diagonal form

$$\mathbf{D} = \text{Diag}(\mathbf{J}_{\lambda_1, n_1}, \dots, \mathbf{J}_{\lambda_L, n_L}) \quad (59)$$

where $\lambda_1, \dots, \lambda_L$ and n_1, \dots, n_L are respectively the distinct eigenvalues of matrix \mathbf{D} and their (algebraic) multiplicities and $\mathbf{J}_{\lambda, n}$ is the standard n -dimensional Jordan block with non-zero entries being $(\mathbf{J}_{\lambda, n})_{i,i} = \lambda$ and $(\mathbf{J}_{\lambda, n})_{i,i+1} = 1$.

Therefore

$$e^{-t\mathbf{D}} = \sum_{i=1}^L \mathbf{U}_i e^{-t\mathbf{J}_{\lambda_i, n_i}} \mathbf{U}_i^T \quad (60)$$

where

$$\mathbf{U}_i = (\mathbf{E}_{N_{i-1}+1}, \dots, \mathbf{E}_{N_i}), \quad N_i = \sum_{k=1}^i n_k \quad (61)$$

is a $N \times n_i$ matrix with columns being the standard coordinate vectors \mathbf{E}_j with entries $E_{j,i} = \delta_{j,i}$ corresponding to the position of the Jordan block $\mathbf{J}_{\lambda_i, n_i}$.

Using (60) and the property that $e^{-t\mathbf{J}_{\lambda, n}} = e^{-t\lambda} e^{-t\mathbf{J}_{0, n}}$, we can write the invariance condition (52) in the following matrix form

$$\sum_{i=1}^L e^{-\lambda_i t} (\mathbf{\Pi} - \mathbf{I}) \mathbf{U}_i e^{-t\mathbf{J}_{0, n_i}} \mathbf{U}_i^T \mathbf{\Pi} = 0, \quad t \geq 0 \quad (62)$$

Since \mathbf{J}_{0, n_i} is a nilpotent matrix of order n_i (i.e. $(\mathbf{J}_{0, n_i})^{n_i} = 0$), we have

$$e^{-t\mathbf{J}_{0, n_i}} = \sum_{k=0}^{n_i-1} \frac{t^k}{k!} (\mathbf{J}_{0, n_i})^k \quad (63)$$

Therefore equation (62) can be written as

$$\sum_{i=1}^L \sum_{k=0}^{n_i-1} \frac{t^k}{k!} e^{-\lambda_i t} (\mathbf{\Pi} - \mathbf{I}) \mathbf{U}_i (\mathbf{J}_{0, n_i})^k \mathbf{U}_i^T \mathbf{\Pi} = 0, \quad t \geq 0 \quad (64)$$

Since $t^k e^{-\lambda_i t}$ are linearly independent functions of t , we get that the following condition should hold for any $i = 1, \dots, L$

$$(\mathbf{\Pi} - \mathbf{I})\mathbf{U}_i (\mathbf{J}_{0,n_i})^k \mathbf{U}_i^T \mathbf{\Pi} = 0, \quad k = 0, \dots, n_i - 1 \quad (65)$$

Note that the Jordan block $\mathbf{J}_{0,n}$ acts as a one position shift to the left

$$\mathbf{J}_{0,n}(a_1, \dots, a_n)^T = (a_2, \dots, a_n, 0)^T \quad (66)$$

Therefore we have for any vector $\mathbf{X} = (X_1, \dots, X_N)^T$

$$\mathbf{U}_i \mathbf{J}_{0,n_i} \mathbf{U}_i^T \mathbf{X} = \sum_{j=N_{i-1}+1}^{N_i-1} X_{j+1} \mathbf{E}_j \quad (67)$$

More generally, for any $k = 0, \dots, n_i - 1$ we have

$$(\mathbf{U}_i \mathbf{J}_{0,n_i} \mathbf{U}_i^T)^k \mathbf{X} = \mathbf{U}_i (\mathbf{J}_{0,n_i})^k \mathbf{U}_i^T \mathbf{X} = \sum_{j=N_{i-1}+1}^{N_i-k} x_{j+k} \mathbf{E}_j \quad (68)$$

Define

$$g_{j,m} = \mathbf{E}_j^T \mathbf{\Pi} \mathbf{E}_m \quad (69)$$

Because $\mathbf{\Pi}$ is an orthogonal projection, $0 \leq g_{j,j} \leq 1$; $g_{j,j} = 0$ is equivalent to $\mathbf{\Pi} \mathbf{E}_j = 0$ and $g_{j,m} = 0$ for all m ; $g_{j,j} = 1$ is equivalent to $\mathbf{\Pi} \mathbf{E}_j = \mathbf{E}_j$ and $g_{j,m} = 0$ for all $m \neq j$.

Proposition 1 *If (65) is satisfied, there exists $0 \leq n_i^* \leq n_i$ such that $g_{j,j} = 1$ for all $N_{i-1} < j \leq N_{i-1} + n_i^*$ and $g_{j,j} = 0$ for all $N_{i-1} + n_i^* < j \leq N_i$.*

Proof. If $g_{j,j} = 0$ for all $N_{i-1} < j \leq N_i$ set $n_i^* = 0$. Otherwise, set

$$n_i^* = \max\{1 \leq j \leq n_i \mid g_{N_{i-1}+j, N_{i-1}+j} \neq 0\} \quad (70)$$

We have by construction that $g_{j,j} = 0$ for all $N_{i-1} + n_i^* < j \leq N_i$. We now prove that $g_{j,j} = 1$ for all $N_{i-1} < j \leq N_{i-1} + n_i^*$.

The case of $n_i^* = 0$ is trivial. Assume $n_i^* > 0$ and denote $j^* = N_{i-1} + n_i^*$. Then $g_{j^*,j^*} > 0$ and $g_{j,m} = 0$ for all $j^* < j \leq N_i$. We will prove by induction with respect to $l = 1, \dots, n_i^*$ that $g_{j,j} = 1$ for all $j = N_{i-1} + l$.

Consider $l = 1$. Multiplying (65) by \mathbf{E}_{j^*} from the right and using the property that $g_{j,m} = 0$ for $j^* < j \leq N_i$, we get

$$(\mathbf{\Pi} - \mathbf{I})\mathbf{U}_i (\mathbf{J}_{0,n_i})^k \mathbf{U}_i^T \sum_{j=N_{i-1}+1}^{j^*} g_{j,j^*} \mathbf{E}_j = 0 \quad (71)$$

Setting $k = n_i^* - 1$ and using (68), we obtain

$$(\mathbf{\Pi} - \mathbf{I})g_{j^*,j^*} \mathbf{E}_{N_{i-1}+1} = 0 \quad (72)$$

Since $g_{j^*,j^*} > 0$, we have $\mathbf{\Pi} \mathbf{E}_{N_{i-1}+1} = \mathbf{E}_{N_{i-1}+1}$ and thus $g_{j,j} = 1$ for $j = N_{i-1} + l$ with $l = 1$.

Suppose we have proved that $g_{j,j} = 1$ for all $N_{i-1} + 1 \leq j \leq N_{i-1} + l$ where $l < n_i^*$. It means that $\mathbf{\Pi} \mathbf{E}_j = \mathbf{E}_j$ for all $N_{i-1} + 1 \leq j \leq N_{i-1} + l$. Consider $N_{i-1} + l + 1 \leq j^*$. Setting $k = n_i^* - l - 1$ in (71) and using (68) we obtain

$$(\mathbf{\Pi} - \mathbf{I}) \left[\sum_{j=N_{i-1}+1}^{N_{i-1}+l+1} g_{j+n_i^*-l-1,j^*} \mathbf{E}_j \right] = 0 \quad (73)$$

Since $\mathbf{\Pi} \mathbf{E}_j = \mathbf{E}_j$ for all $N_{i-1} + 1 \leq j \leq N_{i-1} + l$, we get

$$(\mathbf{\Pi} - \mathbf{I}) g_{j^*,j^*} \mathbf{E}_{N_{i-1}+l+1} = 0 \quad (74)$$

Since $g_{j^*,j^*} > 0$ we get $\mathbf{\Pi} \mathbf{E}_{N_{i-1}+l+1} = \mathbf{E}_{N_{i-1}+l+1}$ and thus $g_{j,j} = 1$ for $j = N_{i-1} + l + 1$. This completes the proof of our proposition by induction.

It follows from Proposition 1 that in the general case of the generating matrix \mathbf{D} defined by its (distinct) eigenvalues $\lambda_1, \dots, \lambda_L$ and their multiplicities n_1, \dots, n_L , the only linear dimensionality reductions preserving the invariance condition (52) are reductions of multiplicities, which also includes dropping some of the eigenvalues by reducing their multiplicities to zero.

Note that we could have obtained this result heuristically from the much simpler case of diagonalizable generating matrix using the fact established in Lyashenko and Goncharov [6, 7] that the sub-basis corresponding to a Jordan block $\mathbf{J}_{\lambda_i, n_i}$ can be approximated with any desirable accuracy by the purely exponential sub-basis defined by a diagonal matrix with n_i distinct eigenvalues that are close enough to λ_i . Thus, dropping some of these distinct, but close to λ_i , eigenvalues would be equivalent to reducing multiplicity of λ_i .