GAUSSIAN-TYPE DENSITY BOUNDS FOR SOLUTIONS TO MULTIDIMENSIONAL BACKWARD SDES AND APPLICATION TO GENE EXPRESSION

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Abstract. We obtain upper and lower Gaussian-type bounds on the density of each component $Y^i_t$ of the solution $Y_t$ to a multidimensional non-Markovian backward SDE. Our approach is based on the Nourdin-Viens formula and a stochastic version of Wazewski’s theorem on the positivity of the components of a solution to an ODE. Furthermore, we apply our results to stochastic gene expression; namely, we estimate the density of the law of the amount of protein generated by a gene in a gene regulatory network.

Keywords: Backward SDEs, Wazewski’s theorem, Nourdin-Viens’ formula, Malliavin Calculus, Stochastic gene expression

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1. Introduction

The aim of this work is to find sufficient conditions to ensure that each component $Y^i_t$ of the solution $Y_t$ to the $m$-dimensional non-Markovian backward SDE (BSDE)

$$Y_t = \xi + \int_t^T g(s, Y_s, Z_s)ds + \int_t^T Z_s dB_s$$

admits a density with respect to Lebesgue measure, and, furthermore, to obtain upper and lower Gaussian-type bounds on this density. In addition, we obtain bounds on tail probabilities. In (1), $B_t$ is an $n$-dimensional Brownian motion and the generator $g : [0, T] \times \Omega \times \mathbb{R}^m \times \mathbb{R}^{m \times n} \to \mathbb{R}^m$ can depend on $\omega$. As a corollary, we obtain Gaussian-type bounds on the components $Y^i_t$ of the solution $Y_t$ to the BSDE

$$Y_t = \varphi(X_T) + \int_t^T g(s, X_s, Y_s, Z_s)ds + \int_t^T Z_s dB_s,$$

where $X_t$ is the solution to the $n$-dimensional SDE

$$X_t = x + \int_0^t f(s, X_s)ds + \int_0^t \sigma(s) dB_s.$$

In (2)-(3), $g : [0, T] \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^{m \times n} \to \mathbb{R}^m$, $f : [0, T] \times \mathbb{R}^n \to \mathbb{R}^n$, and $\sigma : [0, T] \to \mathbb{R}^{n \times n}$ are deterministic functions.

BSDEs have numerous applications in stochastic control theory, mathematical finance, and biology (see, for instance, [4, 13, 23, 25]). Several recent papers studied the existence of densities and density estimates for the laws of solutions to one-dimensional BSDEs [1, 2, 15, 16], fully coupled one-dimensional forward-backward SDEs (FBSDEs) [21], and one-dimensional BSDEs driven by Gaussian processes (in particular, by a fractional Brownian motion) [7]. To the best of our knowledge, the problem of obtaining density estimates for BSDEs in the multidimensional setting...
is addressed for the first time. Furthermore, when density estimates are concerned, each of the above-cited papers deals only with deterministic generators.

To obtain upper and lower Gaussian-type bounds, we use the Nourdin-Viens formula [18]. In the case of one-dimensional SDEs and BSDEs, driven by a one-dimensional Brownian motion, bounds on the density of the solution, say $\mathbb{E}[\int_0^t D_s U_t \mathbb{E}[D_s U_t | \mathcal{F}_s] ds | U_t]$, where $\mathcal{F}_s$ is the (augmented) natural filtration of a one-dimensional Brownian motion. This expression was first introduced in [6]. By extending the approach of [6] to the case of equations driven by a multidimensional Brownian motion, we show that we are required to obtain upper and lower positive deterministic bounds on the expression

$$\mathbb{E}\left[ \int_0^t \sum_{k=1}^n D_s U_t \mathbb{E}[D_s U_t | \mathcal{F}_s] ds | Y_t \right],$$

where $\mathcal{F}_s$ is the (augmented) natural filtration of the $n$-dimensional Brownian motion $B_s$. Unlike the one-dimensional case, where it is usually sufficient to obtain upper and lower positive deterministic bounds on the Malliavin derivative of the solution [1, 6, 18, 21], we aim to obtain a positive lower bound on each component $D_s Y^i_t$ and an upper bound on $|D_s Y^i_t|$. While upper bounds can be obtained by standard techniques, obtaining component-wise lower bounds turns out to be a more delicate task. Our result in this direction is inspired by Wazewski’s theorem on the positivity of the solution components for ODEs [24]. More specifically, we consider the system of linear BSDEs

$$U_t = \xi^i + \int_t^T (K^i_s + \sum_{j=1}^m F^{ij}_s U^j_s + \sum_{j=1}^n G^{ij}_s V^j_s) ds + \sum_{j=1}^n \int_t^T V^{ij}_s dB^j_s,$$

for $i = 1, \ldots, m$. Assuming the non-negativity of $\xi^i$, $K^i_s$ and $F^{ij}_s$ for $i \neq j$, along with additional standard assumptions on the coefficients, we obtain the estimate

$$U_t \geq \mathbb{E}_{Q^i}[e^{\int_t^T F_s^i ds} + \int_t^T e^{\int_t^s F_r^i dr} K_r^i ds | \mathcal{F}_t],$$

where $Q^i$ is a probability measure absolutely continuous with respect to the original measure $\mathbb{P}$. Remark that the existing explicit formulas for solutions to multidimensional linear BSDEs [5, 8] do not allow to obtain component-wise lower bounds.

Note that the $i$-th equation in system (4) depends only on the $i$-th line of the matrix $\{V^{ij}_s\}$. This restricts the class of generators $g(t, y, z)$ to those whose $i$-th component depends only on the $i$-th line of the matrix $z$. However, we provide the following example of a two-dimensional BSDE driven by a one-dimensional Brownian motion:

$$\begin{cases}
Y^1_t = e^{-T} B_T - \int_0^T Z^2_s ds + \int_0^T Z^1_s dB_s, \\
Y^2_t = 2B_T - \cos B_T + \int_0^T Z^2_s dB_s.
\end{cases}$$

For this BSDE we show that (i) for a large interval of values of $t \in (0, T)$, the Malliavin derivative $D_s Y^1_t$ does not take only positive or only negative values; (ii) at some points $t \in (0, T)$, the density of $Y^1_t$ with respect to Lebesgue measure does not possess Gaussian-type bounds. Talking about property (i), we would like to emphasize that the strict positivity of the Malliavin derivative of a random variable (in particular of an SDE or a BSDE solution) is a common requirement to obtaining
Gaussian-type density bounds by means of the Nourdin-Viens formula [18]; see, for instance, [1, 6, 15, 16, 18, 21]. Example (6) shows that the above-described class of generators, i.e., when \( g^i(t, y, z) = g^i(t, y, z^i) \), where \( z^i \) is the \( i \)-th line of the matrix \( z \), is the most general one for which the results on Gaussian-type bounds for one-dimensional BSDEs (e.g. [1, 15, 21]) can be extended to the multidimensional case.

Obtaining Gaussian-type bounds on the densities for the BSDE (2) requires, in particular, lower bounds on the components \( D_k^s X_i^t \) of the Malliavin derivatives of the components of the solution to the forward SDE (3). Since the diffusion coefficient \( \sigma(t) \) is assumed to be independent of the solution \( X_i^t \), \( D_k^s X_i^t \)'s solve a system of ODEs. To obtain non-negative lower bounds on these components, we employ Wazewski’s theorem [24]. Remark that our restriction on the diffusion coefficient is only due to the multidimensional setting. If the forward SDE is one-dimensional, the diffusion coefficient may also depend on \( X_i^t \), and one can apply the Lamperti transform, as it is described, e.g., in [21].

Furthermore, we apply our results to obtain Gaussian-type bounds on the density of the law of the protein level of a gene which is a part of a gene regulatory network. To model stochastic gene expression, we employ the backward SDE approach developed in [23]. Our results apply to a network consisting of more than one gene, and therefore, stochastic gene expression is modeled by a multidimensional BSDE. In addition, we obtain upper and lower bounds on tail probabilities which allows to compute prediction intervals for expression of individual genes. More specifically, in gene expression models, one usually deals with an ensemble of cells, where each cell contains a gene that expresses a certain protein. From this point of view, the protein amount of each gene at time \( t \) becomes a random variable. Thus, one wants to know the interval in which protein amounts of identical genes will fall if we measure them from different cells. Also, using tail probabilities, one can prove that protein amounts remain positive by showing that the probabilities that they are non-positive are negligibly small. Remark that it is not possible to prove that the amounts of proteins are always positive since this would mean that their densities do not possess Gaussian-type bounds.

For one self-regulating gene, whose expression was also modeled by the BSDE method [23], the problem of existence of a density and Gaussian-type bounds on this density was studied in [16]. In addition, in [16], a numerical simulation was performed so one could observe that the density estimates agree with the data produced by the BSDE method. However, the approach used *ibid.* is essentially one-dimensional, and, therefore, can only be applied to a self-regulating gene. Our approach allows to deal with gene regulatory networks. It can also be applied to a self-regulating gene; however, it is not the goal of the present work.

Finally, we performed a numerical simulation for a particular type of a gene regulatory network with the purpose to demonstrate that our density estimates agree with the benchmark data generated by Gillespie’s algorithm [10]. The latter fact, as a byproduct, can be regarded as another evidence of the validity of the BSDE approach [23] as a tool to model stochastic gene expression.

The organization of our paper is as follows. In Section 2, we give some necessary preliminary results. In Section 3, we obtain a “stochastic version” of Wazewski’s theorem; namely, we provide sufficient conditions for the non-negativity of the solution components for linear BSDEs of type (4) and obtain the lower bound (5). In
Section 4, we obtain Gaussian-type bounds on the density of each component $Y^i_t$ of the solution $Y_t$ to both multidimensional BSDEs, (1) and (2). In the same section we demonstrate that if the last argument of $g^i(t, y, z)$ contains not only the $i$-th line of the matrix $z$, then the density of $Y^i_t$ may not have Gaussian-type bounds at some points $t$. Section 5 is dedicated to applications of the theoretical results to gene expression. Namely, we apply the results of Section 4 to obtain Gaussian-type bounds on the density of the law of the amount of protein generated by a gene in a gene regulatory network. Furthermore, using tail probabilities, we compute, theoretically and numerically, prediction intervals for expressions of individual genes. Finally, in the same section, we describe results of a numerical simulation which show that the data obtained by Gillespie’s algorithm fit between the theoretically determined density bound curves.

2. Preliminaries

2.1 Malliavin derivative

Here we describe some elements of the Malliavin calculus that we need in the paper. We refer to [19] for a more complete exposition.

Let $H$ be a real separable Hilbert space and $\mathcal{W}(h)$, $h \in H$, be an isonormal Gaussian process on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, which is a centered Gaussian family of random variables with the property $E(\mathcal{W}(h_1)\mathcal{W}(h_2)) = \langle h_1, h_2 \rangle_H$.

We denote by $\mathcal{D}$ the Malliavin derivative operator. It is known that (see, e.g., [19]) if $F$ is a smooth random variable of the form $F = g(\mathcal{W}(h_1), \ldots, \mathcal{W}(h_k))$, where $g$ is a smooth compactly supported function and $h_i \in H$, $i = 1, \ldots, k$, then

$$DF = \sum_{i=1}^{k} \partial_{x_i} g(\mathcal{W}(h_1), \ldots, \mathcal{W}(h_k))h_i.$$ 

It can be shown that the operator $D$ is closable from the space $S$ of smooth random variables of the above form to $L^2(\Omega, H)$ and can be extended to the space $D^{1,p}$ which is the closure of $S$ with respect to the norm

$$\|F\|_{1,p} = E|F|^p + E\|DF\|_{H}^p.$$ 

In our paper, $H = L_2([0, \infty), \mathbb{R}^n)$ and $\mathcal{W}(h) = \sum_{i=1}^{n} \int_{0}^{\infty} h_i(t)dB^i_t$, where $B^i_t$ are independent real-valued standard Brownian motions.

Furthermore, $\delta$ denotes the Skorokhod integral, and $L = -D\delta$ denotes the Ornstein-Uhlenbeck operator.

2.2 Formula for the density

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. Following [18], we define

$$g_F(x) = E[(D_x F, -D_x L^{-1} F)_H | F = x], \quad x \in \mathbb{R},$$

and recall the criterium for the existence of the density of a real-valued zero-mean random variable $F$ and the explicit formula for this density [18].

**Proposition 1.** Let $F \in D^{1,2}$, $E F = 0$. Then, the law of $F$ has a density $\rho_F$ with respect to Lebesgue measure if and only if $g_F(F) > 0$. In this case, $\text{supp}(\rho_F)$ is a closed interval in $\mathbb{R}$ containing 0 and for almost all $x \in \text{supp}(\rho_F)$

$$\rho_F(x) = \frac{E|F|}{2g_F(x)} \exp \left( - \int_{0}^{x} \frac{y}{g_F(y)} dy \right).$$
Further, in [6], the authors showed that if $\mathcal{H} = L_2([0, \infty), \mathbb{R})$ and the associated isonormal Gaussian process is $W(h) = \int_0^\infty h(t) dB_t$, where $B_t$ is a one-dimensional Brownian motion, then, a.s.,

\begin{equation}
    g_F(F) = \varphi_F(F),
\end{equation}

where $\varphi_F(x) = \mathbb{E} \left[ \int_0^\infty D_r F \mathbb{E}[D_r F | \mathcal{F}_r] dr \right] F = x$, $x \in \mathbb{R}$, and $\mathcal{F}_t$ is the filtration generated by the Brownian motion $B_t$, $t \in \mathbb{R}_+$, and augmented with $\mathbb{P}$-null sets.

3. Positivity of the components of solutions to linear BSDEs

The result of this section is inspired by Wazewski’s theorem [24], and can be regarded as a generalization of the latter to linear backward SDEs.

We start by announcing the Wazewski theorem. Consider the Cauchy problem for a system of linear ordinary differential equations

\begin{equation}
    u'(t) = A(t)u(t), \quad u(0) = u_0, \quad t \in [0, \infty),
\end{equation}

where $A(t)$ is an $n \times n$ matrix. Below, $u^i(t)$ and $u_0^i$ denote the $i$-th coordinates of the vectors $u(t)$ and $u_0$, respectively. The theorem reads:

**Proposition 2.** Let $a_{ij} : [0, \infty) \to \mathbb{R}$ be continuous functions, $i, j = 1, \ldots, n$, and $u(t)$ be the solution to problem (8). Further let $u_0^i \geq 0$ for all $i = 1, \ldots, n$. Then, the following two conditions are equivalent:

1) for all $i, j = 1, \ldots, n$ such that $i \neq j$, $a_{ij}(t) \geq 0$ on $(0, \infty)$;
2) $u^i(t) \geq 0$ for all $t \in (0, \infty)$ and $i = 1, \ldots, n$.

**Corollary 1.** Let the assumptions of Proposition 2 be fulfilled and let condition 1) of the same proposition be in force. Then, for all $i = 0, \ldots, n$ and for all $t \in (0, \infty)$

\begin{equation}
    u^i(t) \geq u_0^i \exp \{ \int_0^t a_{ii}(s)ds \}.
\end{equation}

**Proof.** For the $i$-th coordinate of the solution $u$ we have

\[
    \frac{du^i(t)}{dt} = \sum_{j=1}^n a_{ij}(s)u^j(t) \geq a_{ii}(t)u^i(t).
\]

Indeed, Proposition 2 implies that $\sum_{j \neq i} a_{ij}(t)u^j(t) \geq 0$. Inequality (9) follows now from (the differential from of) Gronwall’s inequality. \hfill $\square$

Note that the backward form of inequality (9) is

\[
    v^i(t) \geq v^i(T) \exp \{ \int_t^T a_{ii}(T - s)ds \}, \quad v^i(t) = u^i(T - t).
\]

We now obtain an analog of Corollary 1, and in particular of the above inequality, for systems of linear BSDEs of the form (4). Let $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbb{P})$ be a filtered probability space, where $\mathcal{F}_t$ is the natural filtration of an $n$-dimensional Brownian motion $B_t$ augmented with $\mathbb{P}$-null sets. Let $U_t$ denote the vector $(U^1_t, \ldots, U^n_t)$ and $V_t$ denote the $\mathbb{R}^{m \times n}$-matrix $\{V^i_{ij}\}_{i,j=1}^m$.

**Theorem 1.** For the coefficients of equation (4) we assume

(i) $F^i_{ij}$, $G^i_t$, $K^i_t$, $i = 1, \ldots, m$, $j = 1, \ldots, n$ are $\mathcal{F}_t$-predictable; $\xi^i \in L_2(\Omega)$ is $\mathcal{F}_T$-measurable; $K^i_t \in L_2(\Omega \times [0, T])$.
Applying Itô’s formula to

Then, for each \( i = 1, \ldots, m \), on \( (\Omega, \mathcal{F}, \mathcal{F}_t) \) there exists a probability measure \( Q^i \), absolutely continuous with respect to \( \mathbb{P} \), such that for each component \( U^i_t \) of the solution to the BSDE (4), estimate (5) holds \( \mathbb{P} \)-a.s.

**Remark 1.** Note that according to [13] (Theorem 2.1), under assumptions (i) and (iii), there exists an \( \mathcal{F}_t \)-adapted pair \((U_t, V_t)\) which solves (4) and such that \( U_t \) is continuous and \( V_t \) is \( \mathcal{F}_t \)-predictable. This pair is unique in the \( L_2(\Omega \times [0, T]) \)-norm.

**Proof of Theorem 1.** Consider the system of BSDEs for \( i = 1, \ldots, m \)

\[
U^i_t = \xi^i + \int_t^T \left( K^i_s + \sum_{j=1,j\neq i}^m F^i_{ij} |U^j_s| + F^i_{ii} U^i_s + (G^i_s, V^i_s) \right) ds + \int_t^T \langle V^i_s, dB_s \rangle, \tag{10}
\]

where \( G^i_t = (G^{i1}_t, \ldots, G^{in}_t) \), \( V^i_t = (V^{i1}_t, \ldots, V^{in}_t) \).

First, let us observe that system (10) also possesses an \( \mathcal{F}_t \)-adapted solution \((U_t, V_t)\) such that \( U_t \) is continuous and \( V_t \) is \( \mathcal{F}_t \)-predictable. This, in particular, follows from the inequality \( ||a| - |b|| \leq |a - b| \), \( a, b \in \mathbb{R} \). Moreover, this pair is unique in the \( L_2(\Omega \times [0, T]) \)-norm (see [13], Theorem 2.1).

Next, by the boundedness of \( G^{ij} \) and the multidimensional version of Girsanov’s theorem (see, e.g., [11], Section 1.7), for each fixed \( i \in \{1, \ldots, m\} \), \( \hat{B}_{t,i} = B_t - \int_0^t G^i_s ds \) is a Brownian motion under the probability measure \( Q^i \) defined as

\[
Q^i\|_{\mathcal{F}_t} = L^i_t \mathbb{P}\|_{\mathcal{F}_t}, \quad L^i_t = \exp \left\{ \int_0^t (G^i_s, dB_s) - \frac{1}{2} \int_0^t |G^i_s|^2 ds \right\}.
\]

Under the probability measure \( Q^i \), the \( i \)-th BSDE in (10) transforms to

\[
U^i_t = \xi^i + \int_t^T \left( K^i_s + \sum_{j=1,j\neq i}^m F^i_{ij} |U^j_s| + F^i_{ii} U^i_s \right) ds + \int_t^T \langle V^i_s, dB_s \rangle, \tag{11}
\]

Applying Itô’s formula to \( e^{\int_0^t F^i_{ii} ds} U^i_t \), noticing that the term \( e^{\int_0^t F^i_{ii} dr} F^i_{ii} U^i_t \) cancels with the equal one, and taking the conditional expectation \( \mathbb{E}_{Q^i}[\cdot \| \mathcal{F}_t] \) with respect to the measure \( Q^i \), we obtain

\[
U^i_t e^{\int_0^t F^i_{ii} ds} = \mathbb{E}_{Q^i} \left[ \xi^i e^{\int_0^T F^i_{ii} ds} + \int_t^T e^{\int_r^T F^i_{ii} dr} (K^i_r + \sum_{j=1,j\neq i}^m F^i_{ij} |U^j_r|) ds \| \mathcal{F}_t \right] \geq \mathbb{E}_{Q^i} \left[ \xi^i e^{\int_0^T F^i_{ii} ds} + \int_t^T e^{\int_r^T F^i_{ii} dr} K^i_r ds \| \mathcal{F}_t \right] \text{ a.s.}
\]

This immediately implies (5) for the solution of the modified BSDE (10). Thus, \( U^i_t \geq 0 \) for all \( i \) a.s., and hence, \( (U^1_t, \ldots, U^m_t) \) is also a solution to (4). By uniqueness, we conclude that (5) holds for all components of the solution to the BSDE (4).

**Corollary 2.** If, under the assumptions of Theorem 1, each \( G^{ij} \) identically equals zero (i.e., the generator does not depend on \( V_t \)), then, in (5), \( Q^i = \mathbb{P} \) for all \( i \).
4. Main result

Let, as before, \((\Omega, \mathcal{F}, \mathcal{F}_t, \mathbb{P})\) be a filtered probability space, where \(\mathcal{F}_t\) is the natural filtration of an \(n\)-dimensional Brownian motion \(B_t\) augmented with \(\mathbb{P}\)-null sets.

Consider the BSDE (1) which we rewrite as a system:

\[
Y^i_t = \xi^i + \int_t^T g^i(s, Y_s, Z_s) ds + \int_t^T (Z^i_s, dB_s), \quad i = 1, \ldots, m.
\]

Here, \(\xi = (\xi^1, \ldots, \xi^m)\) is an \(\mathcal{F}_T\)-measurable random variable, \(g^i\) are components of \(g\), and \(Z^i_t = (Z^i_1, \ldots, Z^i_n)\) is the \(i\)-th line of \(Z_t\). We aim to find sufficient conditions when \(Y^i_t\) possesses a density with respect to Lebesgue measure and find Gaussian-type bounds on this density.

4.1 Gaussian-type density bounds in the situation when the Malliavin derivative is multidimensional

We will need an “\(n\)-dimensional” version of (7). Namely, if \(\mathcal{H} = L_2([0, \infty), \mathbb{R}^n)\) and \(\mathcal{W}(h) = \sum_{i=1}^n \int_0^\infty h_i(t) dB_t^i\), where \(B_t^i\) are independent real-valued standard Brownian motions, then \(g_F(F) = \varphi_F(F)\), where

\[
\varphi_F(x) = E\left[ \int_0^\infty \sum_{i=1}^n D_i^*F E[D_i^*F|\mathcal{F}_s] \ dt \mid F = x \right], \quad x \in \mathbb{R}.
\]

Proposition 3 below is an extension of Proposition 2.3 in [6] to the case of \(\mathcal{H} = L_2([0, \infty), \mathbb{R}^n)\).

**Proposition 3.** Let \(F \in \mathbb{D}^{1,2}\) be a random variable such that \(E[F] = 0\) and \(E \int_0^\infty ||D_i^*F||^2 \ ds < \infty\). Then, \(g_F(F) = \varphi_F(F)\) a.s., where \(\varphi_F(x)\) is defined by (13).

**Proof.** First, we prove that for the covariance \(\text{cov}(F, G)\) of two random variables \(F, G \in \mathbb{D}^{1,2}\), it holds that

\[
\text{cov}(F, G) = E\left[ \int_0^\infty \sum_{i=1}^n D_i^*F E[D_i^*F|\mathcal{F}_s] ds \right].
\]

Remark that in the case \(n = 1\), (14) was obtained in [20] (Proposition 3.4.1). We show (14) for \(n > 1\). By the Clark-Ocone formula (see, e.g., [20], p. 171),

\[
F = EF + \sum_{i=1}^n \int_0^{+\infty} E[D_i^*F|\mathcal{F}_s] dB_s^i.
\]

Therefore,

\[
\text{cov}(F, G) = E\left[ (F - EF)(G - EG) \right] = E\left[ \sum_{i=1}^n \int_0^{+\infty} E[D_i^*F|\mathcal{F}_s] dB_s^i \sum_{i=1}^n \int_0^{+\infty} E[D_i^*G|\mathcal{F}_s] dB_s^i \right] = E\left[ \int_0^{+\infty} \sum_{i=1}^n E[D_i^*F|\mathcal{F}_s] D_i^*G \mid \mathcal{F}_s \right] ds = E\left[ \int_0^{+\infty} \sum_{i=1}^n D_i^*G E[D_i^*F|\mathcal{F}_s] ds \right].
\]

Now by formula (3.15) in [18], for any \(C^1\)-function \(f: \mathbb{R} \to \mathbb{R}\),

\[
\text{cov}(F, f(F)) = E[F f(F)] = E[f'(F)g_F(F)].
\]
Furthermore, for all $x > k$, on the other hand, by (15),

$$
\text{cov} (F, f(F)) = \mathbb{E} \left[ \int_0^\infty \sum_{i=1}^n f'(s)D^i_s F \mathbb{E}[D^i_s F|F_s] \, ds \right] = \mathbb{E}[f'(F)\varphi_F(F)].
$$

Take the function $f(x) = \int_0^x 1_B(y)dy$, where $B \subset \mathbb{R}$ is a Borel set. By approximating $f$ by mollifiers, and then passing to the limit, we obtain the identity $\mathbb{E}[1_B(z)\varphi_F(F)] = \mathbb{E}[1_B(F)\varphi_F(F)]$, or, which is the same, $\int_B g_F(x)\mu_F(dx) = \int_B \varphi_F(x)\mu_F(dx)$, where $\mu_F = \mathbb{P} \circ F^{-1}$. Therefore, $g_F(F) = \varphi_F(F)$ a.s. □

The following corollary will be used for establishing the bounds on the density of $F$ if we know lower bounds on the components $D^k F$ and an upper bound on $|DF|$.}

**Corollary 3.** Let $F \in D^{1,2}$ be $\mathcal{F}_t$-measurable. Assume there exist functions $[0, t] \to (\mathbb{R}^+)^n$, $r \mapsto m_{r,t}$, $(m_{r,t}^1, m_{r,t}^2, \ldots, m_{r,t}^n)$ and $[0, t] \to (0, \infty)$, $r \mapsto M_{r,t}$ such that for each $k = 1, \ldots, n$, $D^k F \geq m_{r,t}^k$ a.s., and, moreover, $|D F| \leq M_{r,t}$ a.s.

Further assume that $\lambda(t) = \int_0^t |m_{r,t}^k|^2 \, dr > 0$ and $\Lambda(t) = \int_0^t M_{r,t}^2 \, dr < \infty$. Then, $F$ admits a density $\rho_F$ w.r.t. Lebesgue measure, and for almost all $x \in \mathbb{R}$,
\[
\frac{\mathbb{E}[F - \mathbb{E}[F]]}{2\Lambda(t)} \exp \left( -\frac{(x - \mathbb{E}[F])^2}{2\Lambda(t)} \right) \leq \rho_F(x) \leq \frac{\mathbb{E}[F - \mathbb{E}[F]]}{2\lambda(t)} \exp \left( -\frac{(x - \mathbb{E}[F])^2}{2\lambda(t)} \right).
\]

Furthermore, for all $x > 0$, the tail probabilities satisfy
\[
\mathbb{P}(F \geq \mathbb{E}[F] + x) \leq \exp \left( -\frac{x^2}{2\lambda(t)} \right) \quad \text{and} \quad \mathbb{P}(F \leq \mathbb{E}[F] - x) \leq \exp \left( -\frac{x^2}{2\Lambda(t)} \right).
\]

**Proof.** By (13), it holds that $\lambda(t) \leq \varphi_F(F) \leq \Lambda(t)$ a.s. By Proposition 3 and Corollary 3.5 in [18], the law of $F$ has a density $\rho_F$ w.r.t. Lebesgue measure and the above estimate for the density $\rho_F$ holds true. The estimates on the tail probabilities follow from Theorem 4.1 in [18]. □

### 4.2 Theorems on Gaussian-type bounds for multidimensional BSDEs

First we would like to ensure the existence and the Malliavin differentiability of the solution to (12). To this end, we introduce assumptions (A1)–(A6) (see [13], Theorem 2.1 and Proposition 5.3):

- **(A1)** $g : [0, T] \times \Omega \times \mathbb{R}^m \times \mathbb{R}^{m \times n} \to \mathbb{R}^m$ possesses uniformly bounded continuous partial derivatives $\partial_\omega g(t, y, z)$ and $\partial_z g(t, y, z)$.
- **(A2)** For each $(y, z), [0, T] \times \Omega \to \mathbb{R}^m$, $(\omega, t) \mapsto g(t, y, z)$ is an $\mathcal{F}_t$-predictable process and $g(\cdot, 0, 0) \in L_2([0, T] \times \Omega)$.

Remark that under (A1) and (A2), there exists an $\mathcal{F}_t$-adapted pair $(Y_t, Z_t)$ solving (12) and such that $Y_t$ is continuous and $Z_t$ is $\mathcal{F}_t$-predictable; the pair is unique with respect to the norm $\mathbb{E}\sup_{[0, T]} |Y_t|^2 + \mathbb{E} \int_0^T |Z_t|^2 \, dt$ (see [13], Theorem 2.1). For the Malliavin differentiability of $(Y_t, Z_t)$, we assume (A3)–(A6) ([13], Proposition 5.3).

- **(A3)** For all $(t, y, z), g(t, y, z) \in D^{1,2}$ and the map $\Omega \times [0, T] \to (L_2([0, T]))^{m \times n}$, $(\omega, t) \mapsto Dg(t, y, z)$ admits an $\mathcal{F}_t$-predictable version.
- **(A4)** $\xi \in L_4(\Omega) \cap D^{1,2}$.
- **(A5)** $\int_0^T |g(s, 0, 0)|^2 \, ds \in L_4(\Omega)$, $Dg(\cdot, 0, 0), Dg(\cdot, Y, Z) \in L_2([0, T]^2 \times \Omega)$.
- **(A6)** For all $(y_1, z_1, y_2, z_2)$ and $t \in [0, T]$,
\[
|D_r g(t, \omega, y_1, z_1) - D_r g(t, \omega, y_2, z_2)| \leq K(t, r, \omega)(|y_1 - y_2| + |z_1 - z_2|)
\]
where for a.e. \( r, K(t, r, \cdot) \) is an \( \mathbb{R}_+ \)-valued \( \mathcal{F}_t \)-adapted process such that 
\( K(\cdot) \in L_4([0, T]^2 \times \Omega) \).

According to [13], Proposition 5.3, under (A1)–(A6), \( Y_t, Z_t \in \mathbb{D}^{1,2} \) and there is a version of \( \{(D^k_t Y_t, D^k_t Z_t), 0 \leq r, t \leq T \} \) satisfying the BSDE

\[
(D^k_t Y_t) = D^k \xi + \int_t^T \left[ D^k_r g(s, Y_s, Z_s) + \partial_y g(s, Y_s, Z_s) D^k_r Y_s \right. \\
+ \partial z g(s, Y_s, Z_s) D^k_r Z_s \left. ds \right] + \int_t^T D^k_r Z_s dB_s \quad \text{if } t \geq r,
\]

and \( D^k_t Y_t = 0, D^k_t Z_t = 0, \) if \( t < r \). Here, \( D^k_r g(s, Y_s, Z_s) = D^k_r g(s, y, z) \big|_{y=Y_s, z=Z_s} \).

Finally, assumptions (A7)–(A10) are necessary to guarantee the existence of a lower bound on each component \( D^k_t Y_t \) and an upper bound on \( |D_r Y_t| \).

(A7) Each component \( g^i(t, y, z) \) of \( g \) depends only on \( z^i = (z^{i1}, \ldots, z^{im}) \) in the last argument.

(A8) There exist non-negative functions \( \beta_k(r), k = 1, \ldots, m, r = 1, \ldots, n, \) with the property \( \int_0^T (\sum_{k=1}^m \beta_k(r)) dr > 0 \) and a positive square-integrable function \( \Phi(r) \) such that a.s. \( D^k_t \xi^i \geq \beta_k(r) \) and \( |D_r \xi| \leq \Phi(r), r \in [0, T] \).

(A9) For all \( t, y, z, r, \) a.s., \( \partial_y g^i(t, y, z) \geq 0 \) for \( i \neq j \).

(A10) There exists a version of \( r \rightarrow D_r g(t, y, z) \) such that for all \( k, i \) and \( r, t \in [0, T] \), a.s., \( D^k_r g^i(t, y, z) \geq 0 \) and \( \mathbb{E} \left[ \int_t^T |D_r g(s, Y_s, Z_s)|^2 ds \right] \mathcal{F}_t \leq \Phi^2(r) \),

where \( \Phi(r) \) is as in (A8).

Theorem 2 and Corollary 4 below are our main results.

**Theorem 2.** Let assumptions (A1)-(A10) be fulfilled. Further let \( Y_t \) be the first component of the unique \( \mathcal{F}_t \)-adapted solution to the BSDE (12) (whose existence is known under (A1) and (A2)). Then, there exists a density \( \rho_{Y^i_t} \) of \( Y^i_t \) w.r.t. Lebesgue measure. Moreover, there are positive functions \( \lambda_i(t), i = 1, \ldots, m, \) and \( \Lambda(t), t \in [0, T], \) that can be computed explicitly, such that for almost all \( x \in \mathbb{R}, \)

\[
\mathbb{E}[|Y^i_t - \mathbb{E}Y^i_t|^2] \leq \mathbb{E}[|Y^i_t - \mathbb{E}Y^i_t|^2] \exp \left( - \frac{x^2}{2\lambda(t)} \right)
\]

Furthermore, for all \( x > 0, \) the tail probabilities satisfy

\[
\mathbb{P}(Y^i_t \geq \mathbb{E}Y^i_t + x) \leq \exp \left( - \frac{x^2}{2\lambda(t)} \right), \\
\mathbb{P}(Y^i_t \leq \mathbb{E}Y^i_t - x) \leq \exp \left( - \frac{x^2}{2\lambda(t)} \right)
\]

To formulate sufficient conditions for the existence of densities and Gaussian-type density bounds for the components of the solution \( Y_t \) to the FBSDE (2)-(3), below we present another set of assumptions, implying (A1)-(A10) for the particular case of \( g \) which becomes random through the dependence on the forward component \( X_t \) of the solution.

(H1) \( f : [0, T] \times \mathbb{R} \rightarrow \mathbb{R} \) possesses a bounded partial derivative \( \partial_x f(t, x) \).
(H2) \( g : [0, T] \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^{m \times n} \to \mathbb{R}^m \), \( g(t, x, y, z) \), possesses bounded continuous partial derivatives \( \partial_x g \) and \( \partial_y g \), and a bounded derivative \( \partial_z g \).

(H3) \( g(\cdot, 0, 0, 0) \in L_2([0, T]) \) and for each \( (y, z) \), \( (t, x) \to g(t, x, y, z) \) is a Borel function.

Note that (H1)–(H3) imply (A1) and (A2) for the BSDE (2). Indeed, under (H1), there exists a unique \( \mathcal{F}_t \)-adapted continuous solution \( X_t \) to (3). Furthermore, there exists an \( \mathcal{F}_t \)-adapted pair \((Y_t, Z_t)\) solving (2) and such that \( Y_t \) is continuous and \( Z_t \) is \( \mathcal{F}_t \)-predictable. The pair is unique with respect to the squared norm \( \mathbb{E} \sup_{[0,T]} |Y_t|^2 + \mathbb{E} \int_0^T |Z_t|^2 dt \) (see [13], Theorem 2.1). We further assume

(H4) \( \sigma \in L_4([0, T]) \).

(H5) \( \varphi \in C^1_0(\mathbb{R}^n \to \mathbb{R}^m) \).

(H6) For all \( (t, x, y_1, z_1, y_2, z_2) \),
\[
|\partial_x g(t, x, y_1, z_1) - \partial_x g(t, x, y_2, z_2)| \leq K(|y_1 - y_2| + |z_1 - z_2|),
\]
where \( K \) is a constant.

Note that \( X_t \in \mathcal{D}^{1,2} \) (see, e.g., [19]). Furthermore, it is straightforward to verify (see the proof of Corollary 4) that (H1)–(H6) imply (A1)–(A6). Therefore, according to [13], \( Y_t, Z_t \in \mathcal{D}^{1,2} \) and there is a version of \( \{(D^k_Y Y_t, D^k_Z Z_t), 0 \leq r, t \leq T\} \) satisfying the BSDE
\[
D^k_Y Y_t = \nabla \varphi(X_T) D^k_X X_T + \int_t^T \left[ \partial_x g(s, X_s, Y_s, Z_s) D^k_X X_s + \partial_y g(s, X_s, Y_s, Z_s) D^k_Z Z_s \right] ds + \int_t^T D^k_Z Z_s dB_s \quad \text{if } t \geq r,
\]
and \( D^k_Y Y_t = 0, D^k_Z Z_t = 0 \), if \( t < r \). Furthermore, \( D^k_x X^i_t \)'s solve the SDE (see [19])
\[
(19)
D^k_x X^i_t = \sigma_{ik}(r) + \sum_{j=1}^n \int_r^t \partial_x \varphi^j(s, X_s) D^k_x X^j_s ds
\]
(written component-wise), where \( \sigma_{ik} \) are the entries of the matrix \( \sigma \). Finally, to guarantee upper and lower bounds for components of \( D_t Y_t \), we assume

(H7) Each component \( g^i(t, x, y, z) \) of \( g \) depends only on \( z = (z^1, \ldots, z^n) \) in the last argument.

(H8) There exist constants \( \gamma_{ij} \geq 0 \) such that \( \partial_{x_j} \varphi^i \geq \gamma_{ij} \) for all \( i = 1, \ldots, m, j = 1, \ldots, n \).

(H9) For all \( (t, x, y, z) \in [0, T] \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^{m \times n} \), \( \partial_y g^i(t, x, y, z) \geq 0 \) for all \( i \neq j \), \( \partial_{x_j} g^i(t, x, y, z) \geq 0 \) for all \( i = j \) and \( \partial_{x_j} g^i(t, x, y, z) \geq 0 \) for all \( i, j \).

(H10) \( \sigma_{ij}(r) \geq 0 \) for all \( i, j \) and \( \sum_{j=1}^n \gamma_{ij}^2 \int_0^r |\sigma_j(r)|^2 dr > 0 \) for all \( i \) and \( t \in (0, T] \), where \( \sigma_j = (\sigma_{j1}, \ldots, \sigma_{jn}) \) is the \( j \)-th line of the matrix \( \sigma \).

**Corollary 4.** Assume (H1)–(H10) and let \( Y_t \) be the second component of the unique \( \mathcal{F}_t \)-adapted solution \((X_t, Y_t, Z_t)\) to the FBSDE (2)–(3) (whose existence is known under (H1)–(H3)). Then, the conclusion of Theorem 2 holds for \( Y_t \).

### 4.3 Gaussian-type bounds may not exist in the absence of (A7) or (H7)

Consider the system of BSDEs (6) which does not satisfy (A7), but satisfies the rest of the assumptions. Below, we show that (i) the Malliavin derivative \( D_t Y_1 \) does not take only positive or only negative values (as \( \omega \) varies) for a large interval
of values of \( t \in (0, T) \); (ii) at some point \( t \in (0, T) \), \( Y_i^1 \) possesses a density with respect to Lebesgue measure, but its density does not have Gaussian-type bounds. Our examples show that the generator satisfying (A7) or (H7) is the most general one for which the results for one-dimensional BSDEs (e.g. [1, 15, 21]) can be extended to the multidimensional case.

**Example 1.** \( D_i Y_i^1 \) takes positive and negative values. Consider the BSDE (6) and let \( T \geq 1 \). The BSDE for Malliavin derivatives (16) for \( t \geq r \) takes the form

\[
\begin{cases}
D_t Y_i^1 = e^{-T} - \int_t^T D_r Z_r^2 ds + \int_t^T D_r Z_r^1 dB_r, \\
D_t Y_i^2 = 2 + \sin B_t + \int_t^T D_r Z_r^2 dB_r.
\end{cases}
\]

In what follows, we will make use of the explicit expressions for the conditional expectations \( \mathbb{E}[\cos B_T \mid \mathcal{F}_t] \) and \( \mathbb{E}[\sin B_T \mid \mathcal{F}_t] \). Applying Itô’s formula to \( e^{z T} \cos B_T \) and \( e^{z T} \sin B_T \) (regarding \( T \) as the time variable), and noticing that two terms in the resulting expressions cancel each other, we obtain

\[
e^{z T} \cos B_T = 1 - \int_0^T e^{z s} \sin B_s dB_s; \quad e^{z T} \sin B_T = \int_0^T e^{z s} \cos B_s dB_s.
\]

Therefore, \( \{e^{z T} \cos B_t\}_{t \geq 0} \) and \( \{e^{z T} \sin B_t\}_{t \geq 0} \) are martingales. This implies

\[
\mathbb{E}[\cos B_T \mid \mathcal{F}_t] = e^{-\frac{z}{2} T} \cos B_t; \quad \mathbb{E}[\sin B_T \mid \mathcal{F}_t] = e^{-\frac{z}{2} T} \sin B_t.
\]

By Proposition 5.3 in [13], \( D_i Y_i \) is a version of \( Z_i \). Therefore, a.s.,

\[
\begin{align*}
Z_i^2 &= 2 + \mathbb{E}[\sin B_T \mid \mathcal{F}_t] = 2 + e^{\frac{z}{2} T} \sin B_t, \\
D_t Z_i^2 &= e^{\frac{z}{2} T} \cos B_t = \mathbb{E}[\cos B_T \mid \mathcal{F}_t], \quad r < t.
\end{align*}
\]

Taking the conditional expectation \( \mathbb{E}[\cdot \mid \mathcal{F}_t] \) in the BSDE for \( D_i Y_i^1 \), by (21), we obtain

\[
D_t Y_i^1 = e^{-T} - \mathbb{E}[\cos B_T \mid \mathcal{F}_t](T - t) = e^{-\frac{z}{2} T} \left(e^{-\frac{z}{2} T} - (T - t)e^{\frac{z}{2} T} \cos B_t\right).
\]

The above formula shows that for \( t \in (0, T - e^{-\frac{z}{2} T}) \), \( D_i Y_i^1 \) takes negative and positive values as \( \omega \) varies; in particular, \( \mathbb{E}[D_i Y_i^1] = e^{-\frac{z}{2} T} \left(e^{-\frac{z}{2} T} - (T - t)\right) \) is negative.

**Example 2. Absence of Gaussian-type bounds on the density of \( Y_i^1 \).** Consider again the BSDE (6) with \( T \geq 1 \). By (20),

\[
Y_i^1(t) = e^{-T} B_t - (2 + \mathbb{E}[\sin B_T \mid \mathcal{F}_t])(T - t)
\]

\[
= -2(T - t) + e^{-T} \left(B_t - e^{\frac{z}{2} T} (T - t) \sin B_t\right).
\]

There exists \( \tau \in (0, T) \) such that \( T - \tau = e^{-\frac{z}{2} T} \). We have

\[
Y_i^1 = \alpha + \beta(B_{\tau} - \sin B_{\tau}), \quad \text{where} \quad \alpha = -2(T - \tau), \quad \beta = e^{-T}.
\]

We show that the density of \( Y_i^1 \) does not possess Gaussian-type bounds. Note that the function \( x \mapsto \alpha + \beta(x - \sin x) \) is strictly increasing. Let \( \psi \) be its inverse function and \( p_\tau(x) = \left(2\pi\tau\right)^{-\frac{1}{2}} \exp\left\{-\frac{x^2}{2\tau}\right\} \) be the Gaussian density. For any bounded measurable function \( \varphi \), we have

\[
\int_{-\infty}^{+\infty} \varphi(\alpha + \beta(x - \sin x)) p_\tau(x) dx = \int_{-\infty}^{+\infty} \varphi(y) \frac{p_\tau(\psi(y))}{\beta(1 - \cos \psi(y))} dy,
\]
where the integration is understood in the Lebesgue sense and the limits on the right-hand side can be computed from the representation \( \psi(y) = \frac{2}{3} - \frac{2}{3} + \sin \psi(y). \)

Thus, the density of \( Y^1_t \) is the function

\[
y \mapsto \frac{p_r(\psi(y))}{\beta(1 - \cos \psi(y))}.
\]

Note that \( p_r(\psi(y)) \) possesses Gaussian-type bounds. However, by the above representation for \( \psi \), the denominator in \( (22) \) takes a countable number of zero values as \( y \rightarrow \pm \infty \) since \( \psi(y) \) reaches all the values \( 2\pi n, n \in \mathbb{N} \). Therefore, the density of \( Y^1_t \) does not possess Gaussian bounds.

4.4 Proofs of Theorem 2 and Corollary 4

Proof of Theorem 2. In order to estimate the density \( \rho_{Y^1_t} \), by Corollary 3, we have to prove the existence of non-negative lower bounds on \( D^k_tY^i_t \) and of an upper bound on \( |D_tY^i_t| \). Under (A7), for each fixed \( k \), the BSDE (16) transforms to

\[
D^k_tY^i_t = D^k_t\xi^i + \int_t^T \left[D^k_r g^i(s, Y^i_s, Z^i_s) + \sum_{j=1}^n \partial_{y^i} g^i(s, Y^i_s, Z^i_s)D^k_rZ^k_j \right] ds + \sum_{j=1}^n \int_t^T D^k_rZ^k_j dB^j_s.
\]

Note that the coefficients of \( (23) \) satisfy the assumptions of Theorem 1. Therefore, for all \( i = 1, \ldots, m \) and \( k = 1, \ldots, n \) it holds that

\[
D^k_tY^i_t \geq \beta_{ik}(r) \exp\{ (T-t) \inf \partial_{y^i} g^i \} = m_{ik}^{r,t}.
\]

For each \( i \), the function \( \lambda_i(t) \) from Corollary 3 can be computed as follows:

\[
\lambda_i(t) = \int_0^t \sum_{k=1}^n \left(m_{ik}^{r,t}\right)^2 dr = \exp\{ 2(T-t) \inf \partial_{y^i} g^i \} \int_0^t \left( \sum_{k=1}^n \beta_{ik}^2(r) \right) dr.
\]

By (A8), \( \lambda_i(t) > 0 \). Let us prove now that for each \( k = 1, \ldots, n \), \( |D^k_tY^i_t| \) is bounded from above a.s. Applying Itô’s formula to \( |D^k_tY^i_t|^2 \) and taking the conditional expectation \( \mathbb{E}[ \cdot | \mathcal{F}_\tau] \) for some \( \tau > 0 \), for all \( t \geq \tau \), from standard estimates and Gronwall’s inequality, we obtain that a.s.

\[
\mathbb{E}[|D^k_tY^i_t|^2 | \mathcal{F}_\tau] \leq \left[ \mathbb{E}[|D^k_\tau|^2 | \mathcal{F}_\tau] + \int_\tau^T \mathbb{E}[|D^k_r g(t, Y^i_t, Z^i_t)|^2 | \mathcal{F}_\tau] dr \right] e^{MT-t}
\]

for some constant \( M > 0 \). Evaluating the above inequality at \( \tau = t \), by (A8) and (A10), we obtain that a.s.,

\[
|D_tY^i_t| \leq C \Phi(r) e^{MT-t}.
\]

Therefore, the function \( \Lambda(t) \) from Corollary 3 is \( \Lambda(t) = 2e^{MT-t} \int_0^t \Phi^2(r) dr \). The statement of the theorem follows now from the aforementioned corollary.

If \( g \) does not depend on \( z \) and \( \omega \), we obtain another bound on \( |D^k_tY^i_t| \) which will be used for a better estimation of tail probabilities in the gene expression model in Section 5.
Lemma 1. Assume \( g \) does not depend on \( z \) and \( \omega \). Then, under the assumptions of Theorem 2, for all \( t \in [0, T] \), a.s.,

\[
|D^k_t Y| \leq \mathbb{E} \left[ \sum_{i=1}^{m} D^k_t \xi^i \mid \mathcal{F}_t \right] \exp \left\{ (T - t) \sup_{j,t,y} \sum_{i=1}^{m} |\partial_{y_i} g^i(t, y)| \right\}.
\]

Proof. Fix \( \tau \in [0, T] \). Summing up the equations in system (23) with respect to \( i \) and taking the conditional expectation with respect to \( \mathcal{F}_\tau \), for all \( t \in [\tau, T] \), we obtain

\[
\mathbb{E} \left[ \sum_{i=1}^{m} D^k_t Y^i_t \mid \mathcal{F}_\tau \right] = \mathbb{E} \left[ \sum_{i=1}^{m} D^k_t \xi^i ds \mid \mathcal{F}_\tau \right] + \int_{\tau}^{T} \mathbb{E} \left[ \sum_{j=1}^{n} \left( \sum_{i=1}^{m} \partial_{y_i} g^i(s, Y^i_s) \right) D^k_r Y^j_r \mid \mathcal{F}_\tau \right] ds.
\]

By the non-negativity of \( D^k_r Y^i_r \) and Gronwall’s inequality, a.s.,

\[
\mathbb{E} \left[ \sum_{i=1}^{m} D^k_r Y^i_r \mid \mathcal{F}_\tau \right] \leq \mathbb{E} \left[ \sum_{i=1}^{m} D^k_t \xi^i \mid \mathcal{F}_\tau \right] \exp \left\{ (T - t) \sup_{j,t,y} \sum_{i=1}^{m} |\partial_{y_i} g^i(t, y)| \right\}.
\]

Since \( |D^k_r Y| \leq \sum_{i=1}^{m} D^k_r Y^i_r \), evaluating the both parts of the above estimate at \( t = \tau \) concludes the proof. \( \square \)

Proof of Corollary 4. We start by obtaining non-negative lower bounds on \( D^k_r X^j_r \). Consider equation (19) for a fixed \( k \in \{1, \ldots, n\} \) and \( j \) varying from 1 to \( n \). By Proposition 1, for all \( j = 1, \ldots, n \) and for all \( t \in (0, T] \),

\[
D^k_r X^j_r \geq \sigma_{jk}(r) \exp \left\{ \int_{\tau}^{T} \partial_{x_j} f^j(s, X^j_s) ds \right\} \geq \sigma_{jk}(r) \exp \{-KT\},
\]

where \( K = \sup_{[0,T] \times \mathbb{R}^n} |\partial_x f(t, x)| \). This is valid for all \( k = 1, \ldots, n \). Also, \( |D_{\tau} X^j | \leq |\sigma(r)| \exp \{KT\} \).

Since \( D^k_r X^j_r \) and \( |D_{\tau} X^j | \) possess the above-mentioned lower and upper bounds, the verification of most of the assumptions of Theorem 2 is straightforward. In particular, since for all \( (y, z) \),

\[
D^k_r g(t, X^j_t, y, z) = \sum_{j=1}^{n} \partial_{x_j} g(t, X^j_t, y, z) D^k_r X^j_r,
\]

where \( \partial_y g \) is bounded, then \( |D^k_r g(t, X^j_t, y, z)| \leq C_1 |\sigma(r)| \) for some constant \( C_1 > 0 \). Furthermore, by the boundedness of the partial derivatives of \( g \), there exists a constant \( C_2 > 0 \) such that

\[
|g(t, x, y, z)| \leq |g(t, 0, 0, 0)| + C_2 (|x| + |y| + |z|).
\]

The above arguments, together with the fact that \( X_t \) possesses moments of all orders, imply (A1)–(A6) and (A10). Furthermore, (A3) holds because for all \( (y, z) \), \( (t, x) \rightarrow \partial_x g(t, x, y, z) \) is a Borel function. Let us show now that assumption (A8) is fulfilled. We have

\[
D^k_r \varphi^i(X_T) = \sum_{j=1}^{n} \partial_{x_j} \varphi^i(X_T) D^k_r X^j_T \geq e^{-KT} \sum_{j=1}^{n} \gamma_{ij} \sigma_{jk}(r) = \beta_{jk}(r),
\]
where \( \beta_{ik}(r) \) are defined by the last expression. By (H10),
\[
\int_0^t \left( \sum_{k=1}^n \beta_{ik}^2(r) \right) dr \geq e^{-2Kt} \sum_{j=1}^n \gamma_{ij}^2 \int_0^t \left( \sum_{k=1}^n \sigma_{jk}^2(r) \right) dr > 0.
\]
On the other hand,
\[
|D_r \varphi(X_T)| \leq |\nabla \varphi(X_T)||D_r X_T| \leq |\sigma(r)| \sup_x |\nabla \varphi(x)| e^{KT}.
\]
This implies (A8).

**Remark 2.** If the forward SDE is one-dimensional, then the diffusion coefficient \( \sigma \) may also depend on \( X_t \), i.e., the SDE can take the form \( X_t = x + \int_0^t f(s, X_s) ds + \int_0^t \sigma(s, X_s) dB_s \). In this case, deterministic non-negative lower and upper bounds for \( D_r X_t \) can be obtained by means of the Lamperti transform (see, e.g., [21]).

5. Application to gene expression

In [23], the authors proposed a BSDE approach to model protein level dynamics for a gene regulatory network. Distributions of proteins, generated by the genes of the network, were represented in the form of histograms which resembled Gaussian-type densities. Here, we aim to prove that under certain assumptions on the parameters of the model, the distributions of proteins indeed possess densities with respect to Lebesgue measure. Moreover, we will use the results of the previous section to obtain upper and lower Gaussian-type bounds on these densities. Furthermore, we compute prediction intervals for expressions of individual genes and show the positivity of amounts of proteins. Finally, we demonstrate how Gaussian-type bounds can be used as a validation tool of the gene expression model. In Subsection 5.2.2, we present a reasonable biological model where upper and lower density bound curves are relatively close to each other and show that these bounds agree with the density profile of benchmark data obtained by Gillespie’s stochastic simulation algorithm (SSA) for modeling of biochemical reactions [10].

5.1 Brief description of the gene expression model

Let \( \eta_t = (\eta_1^t, \ldots, \eta_n^t) \) denote a vector whose \( i \)-th component is the amount of protein generated by gene \( i \). According to [23], the dynamics of \( \eta_t \) is described by the BSDE
\[
\eta_t = \eta_T - \int_t^T f(\eta_s) ds - \int_t^T z_s dB_s, \quad t \in [0, T].
\]
In (27), \( B_t \) is an \( n \)-dimensional Brownian motion, \( \eta_T \) is a given final data (obtained through a simulation using Gillespie’s SSA), and the \( i \)-th component of \( f \) is the synthesis/degradation rate of the \( i \)-th gene which takes the form
\[
f^i(\eta) = \frac{\nu_i}{1 + \exp(-\Theta_i)} - \rho_i \eta^i,
\]
where \( \Theta_i = \sum_{j=1}^n A_{ij} \eta^j \) has the meaning of the total regulatory input to gene \( i \) by other genes of the network. In particular, \( A_{ij} \eta^j \) represents the regulatory effect of gene \( j \) to gene \( i \) with \( A_{ij} \) being the strength of this regulation. Each element \( A_{ij} \) can be negative, positive, or equal zero, indicating repression, activation, or non-regulation, respectively, of gene \( i \) by gene \( j \). Furthermore, \( \nu_i \) denotes the maximum synthesis rate of the \( i \)-th protein, while the same protein degrades at rate \( \rho_i \eta^i \).
final condition \( \eta_T \), determined through a simulation by using Gillespie’s SSA, is represented in the form \( h(B_T) \), where the function \( h : \mathbb{R}^n \to \mathbb{R}^n \) was found in such a way that \( h(B_T) \) matches \( \eta_T \). According to [23], \( h \) looks like a linear function.

The BSDE (27) was solved by means of the associated final value problem for the PDE

\[
\begin{cases}
\partial_t \theta(t, x) + \frac{1}{2} \Delta_x \theta(t, x) - f(\theta(t, x)) = 0, \\
\theta(T, x) = h(x), \quad x \in \mathbb{R}^n,
\end{cases}
\]

and the solution \( \eta_t \) to (27) was computed as \( \theta(t, B_t) \) by means of generating multiple Brownian motion paths.

### 5.2 Bounds on the density and tail probabilities

In what follows, we show how the results obtained in the previous section can be applied to estimate the protein level of a gene in a gene regulatory network.

**Theorem 3.** Let \( \eta_t \) be the solution to the BSDE (27), with the final data \( \eta_T = h(B_T) \). Assume that the partial derivatives of \( h \) satisfy the condition \( \gamma_{ik} \leq \partial_x h^i \leq \Gamma_{ik} \), where \( \Gamma_{ik} \) and \( \gamma_{ik} \geq 0 \) are constants with the property \( \max_k \gamma_{ik} > 0 \) for each \( i \). Further assume that the rate function \( f \) is given by (28) with \( A_{ij} \leq 0 \) for \( i \neq j \).

Then, each component \( \eta_t^i \) of \( \eta_t \) has a density \( \rho_{ij} \) w.r.t. Lebesgue measure. Moreover, estimates (17) and (18) hold with \( Y_t^i = \eta_t^i \) and \( \lambda_i(t), \Lambda(t) \) given by the expressions

\[
\lambda_i(t) = \begin{cases}
|\gamma_i|^2 t \exp\{2(T-t)\rho_i\} & \text{if } A_{ii} \leq 0, \\
|\gamma_i|^2 t \exp\{2(T-t)(\rho_i - \frac{\Delta u}{4})\} & \text{if } A_{ii} > 0,
\end{cases}
\]

\[
\Lambda(t) = t \sum_{k=1}^{n} \left( \sum_{i=1}^{n} \Gamma_{ik} \right)^2 \exp\{2(T-t) \max_j P_j\},
\]

where \( \gamma_i = (\gamma_{i1}, \ldots, \gamma_{in}) \) and

\[
P_j = \sum_{i \neq j} \frac{\nu_i |A_{ij}|}{4} + \max\{\rho_j, |A_{ij}|/4 - \rho_j\}.
\]

**Proof.** First, we note that

\[
\partial_{\eta^i} f^i(\eta) = \psi(\Theta_i) \nu_i A_{ij} - \rho_i \delta_{ij}, \quad \text{where } \psi(x) = \left( \frac{1}{1 + e^{-x}} \right)' = \frac{1}{2(cosh(x) + 1)}.
\]

Furthermore, for all \( r \in [0, T] \),

\[
D^r h^i(B_T) = \partial_{x^i} h^i(B_T) \quad \text{and} \quad D_r h(B_T) = \nabla h(B_T).
\]

We are in the assumptions of Theorem 2, so we conclude that each component \( \eta^i \) has the density w.r.t. Lebesgue measure possessing upper and lower Gaussian-type bounds. Let us compute functions \( \lambda_i(t) \) and \( \Lambda(t) \) from Theorem 2. By (25),

\[
\lambda_i(t) = |\gamma_i|^2 t \exp\{-2(T-t) \sup \partial_{\eta^i} f^i(\eta)\}
\]

which implies (30). Furthermore, by Lemma 1,

\[
|D^r \eta_t| \leq \mathbb{E} \left[ \sum_{i=1}^{n} \partial_{x^i} h^i(B_T) \right] \mathcal{F}_r \exp\left\{ (T-t) \sup \sum_{j=1}^{m} |\partial_{\eta^j} f^j(\eta)|\right\} \leq \left( \sum_{i=1}^{n} \Gamma_{ik} \right) \exp\left\{ (T-t) \max_j P_j\right\},
\]
where $P_j$ is given by (32). Recall that $\Lambda(t) = \int_0^t M^2_{r,t} \, dr$, where $M_{r,t}$ is an upper bound for $|D_r \eta_t|$ (see Corollary 3). This immediately implies (31).

The following corollary is useful for numerical computations in the gene expression model in Subsection 5.3.

Corollary 5. Let the rate function for the gene expression model is as in Theorem 3. Further let the final data are Gaussian and given by $h_i^T(B_T) = c_i B^i_T + b_i$, where $c_i, b_i > 0$, $i = 1, \ldots, n$. Then, the function $\Lambda(t)$ is computed as follows:

$$
\Lambda(t) = t \exp\{2(T - t) \max_j P_j \} \sum_{i=1}^n c_i^2,
$$

where $P_j$ is given by (32).

5.2.1 Prediction intervals and positivity of $\eta^i$

We have the following corollary of Theorem 3.

Corollary 6. Under the assumptions of Theorem 3, the following estimate holds for the $\alpha \cdot 100\%$ prediction interval, where $0 < \alpha < 1$:

$$
P\{ \eta^i_t \in (\mathbb{E}\eta^i_t - x_\alpha, \mathbb{E}\eta^i_t + x_\alpha) \} \geq \alpha,
$$

where $x_\alpha = \sqrt{2\Lambda(t) \ln\left(\frac{2}{1-\alpha}\right)}$ and $\Lambda(t)$ is given by (31).

Proof. Using formulas (18) for tail probabilities, we can evaluate the probability for a prediction interval from above. Namely, for all $x > 0$,

$$
P\{ \eta^i_t \in (\mathbb{E}\eta^i_t - x, \mathbb{E}\eta^i_t + x) \} = 1 - P\{ \eta^i_t \geq \mathbb{E}\eta^i_t + x \} - P\{ \eta^i_t \leq \mathbb{E}\eta^i_t - x \}
\geq 1 - 2 \exp\left( - \frac{x^2}{2\Lambda(t)} \right) = \alpha.
$$

Expressing $x_\alpha$ from the last equation, we obtain (34).

Remark 3. In gene expression models, we usually deal with an ensemble of cells. In our model, each cell contains a gene that expresses the $i$-th protein. The result of Corollary 6 implies that for at least $\alpha \cdot 100\%$ of cells, the amount of the $i$-th protein, which we denote by $\eta^i_t$, lies inside the interval $(\mathbb{E}\eta^i_t - x_\alpha, \mathbb{E}\eta^i_t + x_\alpha)$.

One can use the second inequality in (18) for showing the positivity of $\eta^i_t$'s.

Corollary 7. Under the assumptions of Theorem 3,

$$
P\{ \eta^i_t \leq 0 \} \leq \exp\left( - \frac{(\mathbb{E}\eta^i_t)^2}{2\Lambda(t)} \right).
$$

Note that it is not possible to prove that $\eta^i_t$'s are always positive because this would mean that their densities do not have Gaussian-type bounds. The only way to show this positivity (for the given parameters of the model) is to compute the probability on the right-hand side of (35) and to see whether it is negligibly small.

See Subsections 5.3.2 and 5.3.3 for numerical results related to this subsection.
5.2.2 Precise Gaussian-type bounds for a simplified model

In general, curves representing bounds for the density are not close to each other, so there is not too much information about the real density curve. This happens because obtaining density bounds is related to obtaining upper and lower bounds for the function $\varphi_F$ defined by (13). In some cases, however, it is possible to find more precise Gaussian-type density bounds. This, in particular, allows to see how experimental data (in our case, numerical data obtained by Gillespie’s method) fit between the curves.

We describe a gene regulatory network where we aim to suppress expression of a certain gene, say gene 1. The need to lower expression of specific genes may arise in disease treatment, such as cancer, neurodegenerative diseases, or viral infections [3, 9, 12, 14, 22]. Suppression of gene expression, known as gene silencing or gene knockout, in practice can be achieved by an antisense therapy [17, 22] (when single-stranded short synthetic DNA molecules are delivered inside the cell), genomic editing [3, 14], or administration of antibodies targeting virus gene expression [12].

We model suppression of gene expression by introducing a gene regulatory network, where genes 2, ..., $n$ repress gene 1, while the latter does not regulate the other genes. This means that $A_{1i} < 0$ for all $i = 2, ..., n$. In addition, we assume that each gene activates itself and that genes 2, ..., $n$ do not regulate each other. This implies that $A_{ii} > 0$ for all $i$ and $A_{ij} = 0$ if $i \neq j$ and $i \neq 1$.

By Theorem 3, for the model described above, one can find bounds on the density of the distribution of the first (targeted) protein. Furthermore, for a sufficiently large class of the parameters of the model, one can reasonably estimate the density profile of gene 1. See Subsection 5.3.4 for numerical results, diagrams, and figures based on the results of this subsection.

**Theorem 4.** Let the coefficients $A_{ij}$ and the rate function $f$ be as described above. Then, the first component $\eta^1_t$ of the solution $\eta_t$ to the BSDE (27) with the final data $\eta^i_T = c_iB^i_T + b_i$, $i = 1, ..., n$, where $c_i, b_i > 0$, has a density $\rho_{\eta^1_t}$ w.r.t. Lebesgue measure. Moreover, it holds that

$$\frac{E|\eta^1_t - E\eta^1_t|}{2tM^2_t} \exp\left(-\frac{(x - E\eta^1_t)^2}{2t}\right) \leq \rho_{\eta^1_t}(x) \leq \frac{E|\eta^1_t - E\eta^1_t|}{2tM^2_t} \exp\left(-\frac{(x - E\eta^1_t)^2}{2t}\right),$$

where

$$m_t = c_1 e^{(\rho_1 - \frac{\nu_1 A_{11}}{4})(T-t)}, \quad M_t = e^{\rho_1(T-t)} \sqrt{c_1^2 + \sum_{k=2}^n (\kappa^k_t)^2}$$

with $\kappa^k_t = \nu_1|A_{1k}|e^{\rho_1(T-t)}(T-t)$.

**Proof.** As it was discussed in Subsection 4.2, the BSDE for $D^k_{r}\eta^1_t$ takes the form

$$(36) \quad D^k_{r}\eta^1_t = \delta_{k1}c_1 - \int_t^T \nu_1 \psi(\Theta_1) \sum_{j \neq 1} A_{1j}D^k_{r}\eta^j_s ds$$

$$+ \int_t^T (\rho_1 - \nu_1 \psi(\Theta_1)A_{11})D^k_{r}\eta^1_s ds + \int_t^T D^k_{r}z^1_s dB_s,$$
where \( \psi \) is defined in (33). We claim that if \( k = 1 \), the second term on the right-hand side of (36) equals zero. Indeed, for \( i \neq 1 \),

\[
D^k_r \eta^i_t = \delta_{ki} c_i + \int_t^T (\rho_i - \nu_i \psi(\Theta)) A_{ik} D^k_r \eta^i_s \, ds + \int_t^T D^k_r z^i_s dB_s.
\]

By the equation in (11) (see also Corollary 2),

\[
D^k_r \eta^i_t = \mathbb{E}[\delta_{ki} c_i e^{\int_t^T (\rho_i - \nu_i \psi(\Theta)) ds} | F_t],
\]

which, in particular, implies that \( D^k_r \eta^i_t = 0 \) if \( k \neq i \) and \( i \neq 1 \). Therefore, for \( k = 1 \), the second term on the right-hand side of (36) equals zero. This implies that

\[
D^1_r \eta^i_t = \mathbb{E}[c_1 e^{\int_t^T (\rho_i - \nu_i \psi(\Theta)) ds} | F_t].
\]

Hence, we have the estimate

\[
c_1 e^{(\rho_i - \nu_i) (T-t)} \leq D^1_r \eta^i_t \leq c_1 e^{\rho_i (T-t)}.
\]

Next, if \( k \neq 1 \), by (11) and (36),

\[
D^k_r \eta^i_t = \mathbb{E}\left[\int_t^T e^{\int_t^s (\rho_i - \nu_i \psi(\Theta)) ds} \nu_i \psi(\Theta) A_{ik} | D^k_r \eta^i_s \right] ds | F_t.
\]

Since, by (37), \( 0 < D^k_r \eta^i_t \leq c_k e^{\rho_k (T-t)} \), we obtain the estimate

\[
0 < D^k_r \eta^i_t \leq \frac{\nu_i c_k |A_{ik}|}{4} (T-t) e^{(\rho_i + \rho_k) (T-t)}.
\]

Together with inequalities (38) and Corollary 3, the above estimate implies the statement of the theorem.

\[\square\]

5.3 Numerical results

In this subsection, we compute prediction intervals, the probabilities \( \mathbb{P}\{\eta^i_t \leq 0\} \) (which turn out to be negligibly small), and obtain numerical bounds on the density \( \rho \eta^i_t \) by Theorem 4.

5.3.1 Computation of the expectations \( \mathbb{E}\eta^i_t \) and \( \mathbb{E}|\eta^i_t - \mathbb{E}\eta^i_t| \)

The expectations \( \mathbb{E}\eta^i_t \) and \( \mathbb{E}|\eta^i_t - \mathbb{E}\eta^i_t| \) are computed by the formulas

\[
\mathbb{E}\eta^i_t = \frac{1}{(2\pi t)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \theta^i(t, x) e^{-\frac{|x|^2}{2t}} \, dx,
\]

\[
\mathbb{E}|\eta^i_t - \mathbb{E}\eta^i_t| = \frac{1}{(2\pi t)^{\frac{n}{2}}} \int_{\mathbb{R}^n} |\theta^i(t, x) - \mathbb{E}\eta^i_t| e^{-\frac{|x|^2}{2t}} \, dx,
\]

where \( \theta^i(t, x) \) is the \( i \)-th component of the solution \( \theta(t, x) \) to the final value problem (29) in which the \( i \)-th component of the final condition \( h(x) \) takes the form \( h^i(x) = c_i x_i + b_i \). Above, \( c_i \) and \( b_i \) are positive constants obtained in such a way that the distribution of \( h(B_T) \) coincides with the distribution of \( \eta_T \), where the latter is generated by Gillespie’s method. We aim to find a numerical solution to problem (29) (at time \( t \)) only in the cube \( Q_a = \{x \in \mathbb{R}^n, |x| \leq a\} \) chosen in such a way that in the integrals (39), the integration over \( \mathbb{R}^n \) can be replaced with the integration over \( Q_a \) while keeping the computational error small. Thus, we have to decide how we choose \( a \) and how we obtain a numerical solution to problem (29) in \( Q_a \).

We start by evaluating the parameter \( a \) based on the following two conditions: 1) we make sure that the random variable \( B_T \), when simulated, takes values in \( Q_a \); 2)
we evaluate the error in computing expectations (39) which comes from substituting the actual area of integration by $Q_a$. The probability that $B_T$ is in $Q_a$ can be easily computed. On the other hand, the parameter $a$ can be evaluated by visualizing the simulation of $B_T$ because in practice there are no values of $B_T$ outside of some compact region. Thus, we have to confirm that the error in computing the expectations (39) is small. Note that if $\theta^x_t$ is the solution to the BSDE (27) with the final condition $h(x + B_T - B_T)$, it holds that $\theta^x_t = \theta(\tau, x)$ for all $\tau \in [0, T]$.

We can evaluate $\mathbb{E}[\theta^x_t]$ from the associated BSDE. Indeed, it follows that

$$\mathbb{E}[\theta^x_t] = e^{\rho(T-t)}\mathbb{E}[h_t(x + B_T - B_T)] - \int_t^T e^{\rho(s-t)}\mathbb{E}\left[\frac{\nu_s}{1 + e^{-\nu_s}}\right] ds,$$

where $i$ in the upper index stands for the $i$-th component. Therefore,

$$\theta^i(\tau, x) = e^{\rho(T-\tau)}(c_i x_i + b_i) - \int_\tau^T e^{\rho(s-\tau)}\mathbb{E}\left[\frac{\nu_s}{1 + e^{-\nu_s}}\right] ds.$$

This implies that

$$|\theta^i(t, x)| \leq e^{\rho(T-t)}(c_i |x_i| + b_i + \nu(T-t)).$$

By the first equation in (39), we obtain a bound on $\text{Err} \mathbb{E}\eta^i_t$ by computing the integral of the right-hand side of the above estimate over $\mathbb{R}^n \setminus Q_a$:

$$\text{Err} \mathbb{E}\eta^i_t \leq \frac{1}{(2\pi t)^{\frac{n}{2}}} \int_{\mathbb{R}^n \setminus Q_a} |\theta^i(t, x)| e^{-\frac{|x|^2}{2t}} dx$$

$$\leq e^{\rho(T-t)}(ac_i + c_i(n-1)\sqrt{2\pi} + b_i + \nu) < \frac{1}{2} e^{-z^2}.$$

Finally, we have $\text{Err} \mathbb{E}[\eta^i_t - \mathbb{E}[\eta^i_t]] \leq 2 \text{Err} \mathbb{E}[|\eta^i_t|]$, where $\mathbb{E}[|\eta^i_t|]$ is also estimated by the right-hand side of (40).

To obtain a numerical solution to problem (29) in $Q_a$, we solve the PDE (29) in a larger region, namely in the cube $Q_{a+N}$, while using the boundary condition $\partial \mathbb{E}\eta_t / \partial n \theta(t, x) = 0$, where $n$ is the unit normal vector to the boundary of this cube. This problem is equivalent to the final value problem of the form (29) with the final condition

$$h^i_N(x) = \begin{cases} c_i x_i + b_i & \text{if } |x_i| \leq a + N, \\ c_i(a + N) + b_i & \text{if } x_i > a + N, \\ c_i(-a - N) + b_i & \text{if } x_i < -a - N. \end{cases}$$

We choose $N$ in such a way that the solutions $\theta(t, x)$ and $\theta_N(t, x)$ to the final value problem (29) with the final conditions $h(x)$ and $h_N(x)$ are close enough within $Q_a$. To evaluate this difference, we again use the associated BSDE. By the standard arguments,

$$|\theta(t, x) - \theta_N(t, x)| \leq e^{M(T-\tau)}\left(\mathbb{E}[h(x + B_T - B_T) - h_N(x + B_T - B_T)]^2\right)^{\frac{1}{2}},$$

where $M$ is a bound on $\nabla f$, which can be computed using expression (28). For this bound, one can take, for example, $M = \sqrt{\sum 2m_i^2}$, where $m_i = \max\{\rho_i, \nu_i |A_i|\}$ and $|A_i| = \sqrt{\sum_{j=1}^n A^2_{ij}}$. Using the explicit form of $h$ and $h_N$, we compute the right-hand
side of the above inequality, which gives

\[
\sup_{x \in Q_0} |\theta(t, x) - \theta_N(t, x)| \leq \frac{|c|(T - \tau)^{3/2}}{N^{3/2}} e^{M(T-\tau) - \frac{\sqrt{N}}{\tau}}.
\]

where \( c = (c_1, \ldots, c_n) \). Thus, we consider \( \theta_N(t, x) \) as a numerical solution to problem (29) in \( Q_0 \). To obtain \( \theta_N \), problem (29) was transformed to an initial problem by the time change \( t \leftrightarrow T - t \). The resulting system of PDEs with the initial condition \( h_N(x) \) and the boundary condition \( \partial_n \theta = 0 \) was solved by the fractional step Crank-Nicolson scheme in each spatial direction.

5.3.2 Computation of prediction intervals

We computed prediction intervals using the formulas obtained in Corollary 6. We considered a network of three fully interacting genes with the final data \( h_i(B_T) = c_iB_T^i + b_i, i = 1, 2, 3 \) and the following set of parameters: \( T = 6, t = 3, c_1 = 5, c_2 = 0.5, c_3 = 0.3, b_1 = 150, b_2 = 70, b_3 = 80, \nu_1 = 0.5, \nu_2 = 0.75, \nu_3 = 1.0, \rho_1 = 0.2, \rho_2 = 0.5, \rho_3 = 0.6 \), and the matrix \( A = \{A_{ij}\} \) given by

\[
A = \begin{pmatrix}
2.5 & -0.2 & -0.25 \\
-0.03 & 3.0 & -0.3 \\
-0.5 & -0.1 & 2.0
\end{pmatrix}.
\]

We obtained

\[
\mathbb{P}\{\eta^1 \in (129.8, 409.5)\} \geq 0.75; \quad \mathbb{P}\{\eta^1 \in (83.4, 455.9)\} \geq 0.95;
\]
\[
\mathbb{P}\{\eta^2 \in (157.7, 437.4)\} \geq 0.75; \quad \mathbb{P}\{\eta^2 \in (111.3, 483.8)\} \geq 0.95;
\]
\[
\mathbb{P}\{\eta^3 \in (311.7, 591.4)\} \geq 0.75; \quad \mathbb{P}\{\eta^3 \in (265.3, 637.8)\} \geq 0.95.
\]

5.3.3 Positivity of \( \eta^i \)

In the situation described in the previous subsection, in particular, using the same set of parameters, we obtained the estimates on probabilities of the events that the components of \( \eta^i \) are non-positive:

\[
\mathbb{P}\{\eta^1 \leq 0\} \leq 4 \cdot 10^{-4}; \quad \mathbb{P}\{\eta^2 \leq 0\} \leq 8 \cdot 10^{-5}; \quad \mathbb{P}\{\eta^3 \leq 0\} \leq 4 \cdot 10^{-10}.
\]

This confirms that each \( \eta^i \) is positive. In [23], the positivity of \( \eta^i \) is a result of agreeing of the BSDE method with Gillespie’s SSA and the fact that the final condition \( \eta^i_T \), provided by SSA, was modeled as \( c_iB_T^i + b_i \) by fitting the parameters \( c_i \) and \( b_i \). Here, for the same purpose, we use the result of Subsection 5.2.1.

5.3.4 Numerical bounds on the density in the simplified model

For the model described in Subsection 5.2.2, we performed two simulations with different sets of parameters; the number of genes in both simulations was taken three. The first simulation was performed with the following parameters: \( \rho_1 = \rho_2 = \rho_3 = 1; \nu_1 = 0.4, \nu_2 = 0.1, \nu_3 = 0.3; c_1 = 4.89, c_2 = 0.47, c_3 = 0.51, b_1 = 75.98, b_2 = 7.84, b_3 = 8.85; A_{11} = 0.1, A_{22} = 0.04, A_{33} = 0.6, A_{12} = A_{13} = -2, A_{ij} = 0 \) if \( i \neq j \) and \( i \neq 1 \); \( T = 4 \) and \( t = 2 \). Here, the role of the second and the third genes in repressing the first gene is not so significant. The self-degradation of the first gene plays a bigger role compared to the other simulation. The second simulation was performed with the parameters: \( \rho_1 = 0.05, \rho_2 = \rho_3 = 10^{-4}; \nu_1 = 5, \nu_2 = 1, \nu_3 = 1; c_1 = 1, c_2 = 10^{-2}, c_3 = 10^{-2}, b_1 = 55.32, b_2 = 712.34, b_3 = 834.02; A_{11} = 10^{-5}, A_{22} = 10^{-2}, A_{33} = 0.1, A_{12} = -4, A_{13} = -3.5, A_{ij} = 0 \) if \( i \neq j \) and \( i \neq 1 \); \( T = 18 \).
and \( t = 9 \). Here, the second and the third genes play a bigger role in repressing the first gene. This happens because \( \Theta_1 = A_{11} \eta_1 + A_{12} \eta_2 + A_{13} \eta_3 \) is a big negative number reducing the synthesis rate of the first protein according to formula (28), and thus, allowing it to degrade.

The density bound curves were computed by Theorem 4; specifically, by computing the expressions for \( m_t \) and \( M_t \), and the expectations \( \mathbb{E}_{\eta_1^t} \) and \( \mathbb{E} |\eta_1^t - \mathbb{E}_{\eta_1^t}| \).

Furthermore, we performed a simulation using Gillespie’s SSA. First of all, we did it to obtain the parameters \( c_i \) and \( b_i \), \( i = 1, 2, 3 \) (in such a way that the distributions of \( \eta_i^T \) and \( c_i B_i^T + b_i \) coincide), but also, to demonstrate that our density estimates agree with the data generated by SSA. To verify the latter, we plotted a histogram (in green, see the figures) obtained by SSA and observed that it fits quite well between the curves computed by using Theorem 4. Remark that obtaining the aforementioned density bounds is fully based on the BSDE (27) which is in the heart of the BSDE method introduced in [23]. By this, the validity of this method is confirmed once again.

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