Backward martingale transport and Fitzpatrick functions in pseudo-Euclidean spaces

Dmitry Kramkov* and Mihai Sirbu†

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Abstract

We study an optimal transport problem with a backward martingale constraint in a pseudo-Euclidean space $S$. We show that the dual problem consists in the minimization of the expected values of the Fitzpatrick functions associated with maximal $S$-monotone sets. An optimal plan $\gamma$ and an optimal maximal $S$-monotone set $G$ are characterized by the condition that the support of $\gamma$ is contained in the graph of the $S$-projection on $G$. For a Gaussian random variable $Y$, we get a unique decomposition: $Y = X + Z$, where $X$ and $Z$ are independent Gaussian random variables taking values, respectively, in complementary positive and negative linear subspaces of the $S$-space.

Keywords: martingale optimal transport, pseudo-Euclidean space, Fitzpatrick function.

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* Carnegie Mellon University, Department of Mathematical Sciences, 5000 Forbes Avenue, Pittsburgh, PA, 15213-3890, USA, kramkov@cmu.edu. The author also has a research position at the University of Oxford.

† The University of Texas at Austin, Department of Mathematics, 2515 Speedway Stop C1200, Austin, Texas 78712, sirbu@math.utexas.edu. The research of this author was supported in part by the National Science Foundation under Grant DMS 1908903.
1 Introduction

Let $S$ be a symmetric $d \times d$ matrix with full rank and $m$ positive eigenvalues. The bilinear form

$$S(x, y) := \langle x, S y \rangle = \sum_{i,j=1}^{d} x^i S_{ij} y^j, \quad x, y \in \mathbb{R}^d,$$

defines the scalar product on a pseudo-Euclidean space $\mathbb{R}^d_m$ with dimension $d$ and index $m$, which we call the $S$-space. The quadratic form $S(x, x)$ is called the scalar square; its value may be negative.

Given a Borel probability measure $\nu$ on $\mathbb{R}^d$ with finite second moments, we study the backward martingale transport problem:

$$\max \int \frac{1}{2} S(x, y) d\gamma \quad \text{over} \quad \gamma \in \Gamma(\nu), \quad (1)$$

where $\Gamma(\nu)$ is the family of Borel probability measures $\gamma = \gamma(dx, dy)$ on $\mathbb{R}^{2d}$ having $\nu$ as their $y$-marginal and the martingale property: $\gamma(y|x) = x$. Contrary to the usual setup of optimal transport, with or without the martingale constraints, the $x$-marginal of $\gamma$ is not an input, but a part of the solution. In the case $m = 1$ and $S$ given by (2), problem (1) has been studied in [14], where it was motivated by an application from financial economics.

We point out that the problem of unconstrained optimal transport with given $x$-marginal $\mu$ and the quadratic cost function $c(x, y) = -S(x, y)$ can be reduced to the classical $L^2(\mathbb{R}^d)$-framework of [5] by a linear transformation. The same problem with a martingale constraint is trivial, as

$$\int S(x, y) d\gamma = \int S(x, x) d\mu.$$

For nonquadratic cost functions, such martingale optimal transport has been the subject of intensive research, see, for example, [2, 3, 4, 11], and [9].

Our main Theorem 2.5 states that $\gamma$ is an optimal plan for (1) if and only if its support is contained in the $y$-based graph of the projection multifunction

$$P_G(y) := \arg \min_{x \in G} S(x - y, x - y), \quad y \in \mathbb{R}^d,$$

on a maximal $S$-monotone set $G$. Here, a set $G \subset \mathbb{R}^d$ is called $S$-monotone or $S$-positive if

$$S(x - y, x - y) \geq 0, \quad x, y \in G,$$
Figure 1: The convex set $Q_G(x) \subset P^{-1}_G(x)$ contains the points $y_i, i = 1, 2$. Hyperbola $H_i$ with focus at $y_i$ is tangent to $G$ at $x$.

and maximal $S$-monotone, if it is not a strict subset of an $S$-monotone set. If $d = 2m$ and the matrix $S$ has the form:

$$S = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

where $I$ is the $m$-dimensional identity matrix, then the $S$-monotonicity becomes the classical monotonicity: see, for example, [19, p. 240]. Geometrically, $P_G(y)$ consists of those $x \in G$ where the hyperboloid

$$H_G(y) := \left\{ z \in \mathbb{R}^d \mid S(y - z, y - z) = \min_{w \in G} S(y - w, y - w) \right\}$$

is tangent to $G$, as in Figure 1. If $x \in P_G(y)$, then the vector $y - x$ is $S$-normal to $G$ at $x$ in the sense that

$$\limsup_{z \to x, z \in G} \frac{S(y - x, z - x)}{|z - x|} \leq 0.$$

The map $y \to P_G(y) \ni x$ taking values in the closed subsets of $G$ describes the backward evolution of the canonical martingale $(x, y)$ under $\gamma$. In terms of the forward evolution, an optimal plan is characterized as

$$x \in G, \quad y \in Q_G(x), \quad \gamma - a.s.,$$

where $Q_G(x)$ is the smallest closed convex subset of

$$P^{-1}_G(x) := \{ y \in \mathbb{R}^d \mid P_G(y) = x \}$$
containing \( x \) in its relative interior. If \( y \in Q_G(x) \), then the vector \( y - x \) is \( S \)-orthogonal to \( G \) at \( x \) in the sense that

\[
\lim_{z \to x, z \in G} \frac{S(y - x, z - x)}{|z - x|} = 0.
\]

The associated dual problem to (1) turns out to be

\[
\text{minimize } \int \psi_G(y) d\nu \quad \text{over } \ G \in \mathcal{M}(S),
\]

where \( \mathcal{M}(S) \) is the family of all maximal \( S \)-monotone sets and

\[
\psi_G(y) := \sup_{x \in G} \left( S(x, y) - \frac{1}{2} S(x, x) \right), \quad y \in \mathbb{R}^d.
\]

For \( S \) given by (2), \( \psi_G \) is the classical Fitzpatrick function from convex analysis, see [7] and [17]. We shall use this term also for general \( S \)-spaces. The Fitzpatrick functions \( \psi_G \) play in our analysis the role of the Kantorovich potentials from unconstrained optimal transport. Monotone sets in \( S \)-spaces and their corresponding Fitzpatrick functions have been introduced in [20] and further studied in [16].

Problems (1) and (2) can be solved explicitly if \( \nu \) is the law of a Gaussian random variable \( Y \) with positive definite covariance matrix \( \Sigma \). Theorem 4.5 shows that the optimal plan \( \gamma \) for (1) is given by the law of \((X,Y)\), where \( X \) is the unique random variable such that \( X \) and \( Z := Y - X \) are independent Gaussian and their respective supports are complementary positive and negative linear subspaces of the \( S \)-space:

\[
S(X, X) \geq 0, \quad S(Z, Z) \leq 0, \quad S(X, Z) = 0.
\]

The covariance matrices \( Q \) for \( X \) and \( R \) for \( Z \) are uniquely defined by the conditions:

\[
\Sigma = Q + R, \quad QSQ \geq 0, \quad RSR \leq 0, \quad QSR = 0,
\]

where inequalities mean that the respective matrices are positive and negative semi-definite.

The original motivation for the backward martingale transport comes from the Kyle’s equilibrium for insider trading introduced in [15]. For \( m = 1 \)
and $S$ given by (2), the paper [14] provides sharp conditions for the existence and uniqueness of a version of such equilibrium from [18]. Our main Theorem 2.5 sets up the base for an extension of these criteria to higher dimensions.

Our results also provide pseudo-Euclidean counterparts to the solutions of the classical problems of linear and nonlinear PCA (principal component analysis). The optimal linear hyperplane $G = \text{range } Q$ given by Theorems 4.5 and 4.1 is the PCA fit of the multivariate Gaussian distribution in the $S$-space: $G$ is the span of the eigenvectors corresponding to the largest (equivalently, positive) $m$ eigenvalues of the characteristic equation \( \det(S - \lambda \Sigma^{-1}) = 0 \). The optimal maximal $S$-monotone set $G$ from Theorem 2.5 is a pseudo-Euclidean version of a self-consistent or principle curve from [10]. Notice that being maximal $S$-monotone, the set $G$ is a maximal Euclidean-type subset of $\mathbb{R}^d$ in the $S$-space: $S(x - y, x - y) \geq 0, \ x, y \in G$. As a result, $G$ has qualitative properties of a standard Euclidean PCA fit.

For both applications above, it is important to know whether an optimal plan $\gamma$ admits the map representation: there is a Borel function $f$ on $\mathbb{R}^d$ such that

$$x = f(y), \quad \gamma(dx, dy) - a.s.$$

The follow-up paper [13] contains sharp conditions for the existence of such representation as well as for the uniqueness of an optimal plan $\gamma$.

The current paper is organized as follows. The existence and characterizations of an optimal plan $\gamma$ and an optimal set $G$ are established in Theorem 2.5 in Section 2. Properties of optimal $\gamma$ and $G$ are collected in Section 3. The linear case is studied in Section 4. Finally, Appendix A lists the main features of $S$-Fitzpatrick functions.

**Notation**

The scalar product and the norm in the Euclidean space $\mathbb{R}^d$ are written as

$$\langle x, y \rangle := \sum_{i=1}^d x_i y_i, \quad |x| := \sqrt{\langle x, x \rangle}, \quad x, y \in \mathbb{R}^d.$$ 

For a Borel probability measure $\mu$ on $\mathbb{R}^d$, a $\mu$-integrable $m$-dimensional Borel function $f = (f_1, \ldots, f_m)$, and an $n$-dimensional Borel function $g = \ldots$
(g_1, \ldots, g_n), the notation $\mu(f|g)$ stands for the $m$-dimensional vector of conditional expectations of $f_i$ given $g$ under $\mu$:

$$
\mu(f|g) = (\mu(f_1|g_1, \ldots, g_n), \ldots, \mu(f_m|g_1, \ldots, g_n)).
$$

In particular, we write $\mu(f)$ for the vector of expected values:

$$
\mu(f) = \int f \, d\mu = (\int f_1 d\mu, \ldots, \int f_m d\mu) = (\mu(f_1), \ldots, \mu(f_m)).
$$

We write $\text{supp } \mu$ for the support of $\mu$, the smallest closed set of full measure. For $p \geq 1$, we denote by $\mathcal{P}_p(\mathbb{R}^d)$ the family of Borel probability measures $\mu$ on $\mathbb{R}^d$ such that $\mu(|x|^p) = \int |x|^p \, d\mu < \infty$.

For a closed (equivalently, lower semi-continuous) convex function $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, we denote by $\partial f$ its subdifferential and by $f^*$ its convex conjugate:

$$
\partial f(x) = \{ z \in \mathbb{R}^d \mid f(y) - f(x) \geq \langle z, y - x \rangle, \ y \in \mathbb{R}^d \}, \quad x \in \mathbb{R}^d,
$$

$$
f^*(y) := \sup_{x \in \mathbb{R}^d} (\langle y, x \rangle - f(x)), \quad y \in \mathbb{R}^d.
$$

We recall that, [19], Theorem 23.5, p. 218,

$$
f(x) = \langle x, y \rangle - f^*(y) \iff y \in \partial f(x) \iff x \in \partial f^*(y), \quad x, y \in \mathbb{R}^d. \quad (3)
$$

The domains of $f$ and of $\partial f$ are defined as

$$
\text{dom } f := \{ x \in \mathbb{R}^d \mid f(x) < \infty \},
$$

$$
\text{dom } \partial f := \{ x \in \text{dom } f \mid \partial f(x) \neq \emptyset \}.
$$

# 2 Backward martingale transport

We denote by $S_m^d$ the family of symmetric $d \times d$-matrices of full rank with $m \in \{0, 1, \ldots, d\}$ positive eigenvalues. For $S \in S_m^d$, the bilinear form

$$
S(x, y) := \langle x, Sy \rangle = \sum_{i,j=1}^d x_i S_{ij} y_j, \quad x, y \in \mathbb{R}^d,
$$

defines the scalar product on a pseudo-Euclidean space $\mathbb{R}_m^d$ with dimension $d$ and index $m$, which we call the $S$-space. The quadratic form $S(x, x)$ is called the scalar square; its value may be negative.
We view a point \((x, y)\) in the product space \(\mathbb{R}^{2d} = \mathbb{R}^d \times \mathbb{R}^d\) as the initial and terminal values of the canonical \(d\)-dimensional process. Given the terminal law \(\nu = \nu(dy) \in \mathcal{P}_2(\mathbb{R}^d)\), our goal is to

\[
\text{maximize } \frac{1}{2} \int S(x, y) d\gamma \text{ over } \gamma \in \Gamma(\nu), \tag{4}
\]

where \(\Gamma(\nu)\) is the family of Borel probability measures \(\gamma = \gamma(dx, dy) \in \mathcal{P}_2(\mathbb{R}^{2d})\) having \(\nu\) as their \(y\)-marginal and making a martingale out of the canonical process:

\[
\Gamma(\nu) := \{ \gamma \in \mathcal{P}_2(\mathbb{R}^{2d}) \mid \gamma(\mathbb{R}^d, dy) = \nu(dy) \text{ and } \gamma(y|x) = x \}.
\]

The martingale property of \(\gamma \in \Gamma(\nu)\) yields that

\[
\int S(x, y) d\gamma = \int S(x, x) d\gamma,
\]

\[
\int S(x - y, x - y) d\gamma = \int S(y, y) d\nu - \int S(x, y) d\gamma.
\]

Thus, the problem (4) is equivalent to the minimization of the expected value of the scalar square between \(x\) and \(y\) over \(\Gamma(\nu)\):

\[
\text{minimize } \int S(x - y, x - y) d\gamma \text{ over } \gamma \in \Gamma(\nu). \tag{5}
\]

Theorem 3.2 contains another reformulation of (4).

A set \(G \subset \mathbb{R}^d\) is called \(S\)-monotone or \(S\)-positive if

\[
S(x - y, x - y) \geq 0, \quad x, y \in G,
\]

that is, if the restriction to \(G\) of the scalar square takes values in \([0, \infty)\). An \(S\)-monotone set \(G\) is called maximal if it is not a strict subset of an \(S\)-monotone set. Theorem 2.5 shows that a dual problem to (4) is to

\[
\text{minimize } \int \psi_G(y) d\nu \text{ over } G \in \mathfrak{M}(S), \tag{6}
\]

where \(\mathfrak{M}(S)\) is the family of all maximal \(S\)-monotone sets and

\[
\psi_G(y) := \sup_{x \in G} \left( S(x, y) - \frac{1}{2} S(x, x) \right), \quad y \in \mathbb{R}^d,
\]
is a closed convex function taking values in $\mathbb{R} \cup \{+\infty\}$. For general quadratic forms $S$ such function $\psi_G$ was introduced in [20]. We call $\psi_G$ a Fitzpatrick function because of Example 2.3. We collect the basic properties of Fitzpatrick functions in the $S$-space in Appendix A.

**Example 2.1.** If $S \in \mathcal{S}_d$, that is, $S$ is positive definite:

$$S(x, x) = \langle x, Sx \rangle > 0, \quad x \neq 0,$$

then $G = \mathbb{R}^d$ is the only element of $\mathcal{M}(S)$ and

$$\psi_G(y) = \sup_{x \in \mathbb{R}^d} \left( S(x, y) - \frac{1}{2} S(x, x) \right) = \frac{1}{2} S(y, y), \quad y \in \mathbb{R}^d.$$

Trivially, $G = \mathbb{R}^d$ is the optimal set for (6). From (5) we deduce that $x = y$, $\gamma - a.s.$, under the optimal plan $\gamma$ for (4).

**Example 2.2.** If $S \in \mathcal{S}_0^d$, that is, $S$ is negative definite:

$$S(x, x) = \langle x, Sx \rangle < 0, \quad x \neq 0,$$

then all maximal $S$-monotone sets are points: $\mathcal{M}(S) = \mathbb{R}^d$. If $G = \{x\}$, where $x \in \mathbb{R}^d$, then

$$\psi_G(y) = S(x, y) - \frac{1}{2} S(x, x), \quad y \in \mathbb{R}^d.$$

Elementary computations show that the optimal set $G$ for (6) is given by $\{\nu(y)\}$ and that $x = \nu(y)$, $\gamma - a.s.$, under the optimal plan $\gamma$ for (4).

**Example 2.3.** If $d = 2m$ and $S$ has the form (2), that is,

$$S(x, y) = \sum_{i=1}^{m} (x^i y^{m+i} + x^{m+i} y^i), \quad x, y \in \mathbb{R}^{2m},$$

then $S \in \mathcal{S}_m^{2m}$, the $S$-monotonicity means the standard monotonicity in $\mathbb{R}^{2m} = \mathbb{R}^m \times \mathbb{R}^m$, and $\psi_G$ becomes the classical Fitzpatrick function from [7]. For $d = 2$, problems (4) and (6) have been studied in [14], where they were motivated by applications in financial economics.
Example 2.4. If $S$ is the canonical quadratic form in $S_m^d$: 
\[
S(x, y) = \sum_{i=1}^{m} x_i y_i - \sum_{i=m+1}^{d} x_i y_i, \quad x, y \in \mathbb{R}^d,
\]
then a set $G$ is $S$-monotone if and only if 
\[
G = \text{graph } f := \{(u, f(u)) \mid u \in D\},
\]
where $D \subset \mathbb{R}^m$ and $f : D \to \mathbb{R}^{d-m}$ is a 1-Lipschitz function: 
\[
|f(u) - f(v)| \leq |u - v|, \quad u, v \in D.
\]
By the Kirszbraun Theorem, [6, 2.10.43], every 1-Lipschitz function can be extended to the whole $\mathbb{R}^m$. It follows that $G \in \mathcal{M}(S)$ if and only if it is the graph of a global 1-Lipschitz function $f : \mathbb{R}^m \to \mathbb{R}^{d-m}$.

Let $G \in \mathcal{M}(S)$. The Fitzpatrick function $\psi_G$ is closely related to the minimization of the scalar square relative to $G$: 
\[
\phi_G(y) := \inf_{x \in G} S(x - y, x - y) = S(y, y) - 2\psi_G(y), \quad y \in \mathbb{R}^d.
\]
Theorem A.4 yields that $x \in G$ and $y \in \partial\psi_G^*(Sx)$ (equivalently, $Sx \in \partial\psi_G(y)$) if and only if $x$ is a projection of $y$ on $G$ in the $S$-space: 
\[
x \in P_G(y) := \arg \min_{z \in G} S(y - z, y - z)
= \left\{ z \in G \mid S(y - z, y - z) = \phi_G(y) \right\}
= \left\{ z \in G \mid \psi_G(y) = S(y, z) - \frac{1}{2}S(z, z) \right\}. \tag{7}
\]
The inverse image of $P_G$ has the form: 
\[
P_G^{-1}(x) := \left\{ y \in \mathbb{R}^d \mid x \in P_G(y) \right\} = \partial\psi_G^*(Sx), \quad x \in G,
\]
and thus, takes values in the convex closed sets. Geometrically, $x \in P_G(y)$ if and only if the hyperboloid 
\[
H_G(y) := \left\{ z \in \mathbb{R}^d \mid S(y - z, y - z) = \phi_G(y) \right\}
\]
is tangent to $G$ at $x$. Figure 1 provides an illustration for $d = 2$ and $S = S(x, y)$ from Example 2.3.
Theorems 2.5 and 3.1 show that the geometric properties of an optimal plan for (4) are fully described by the multi-function

\[ Q_G(x) := \bigcup_{n \geq 1} Q_G^{1/n}(x), \quad x \in G, \]

where for \( \epsilon > 0 \)

\[ Q_G^\epsilon(x) := \{ y \in P_G^{-1}(x) \mid x + \epsilon(x - y) \in P_G^{-1}(x) \}, \quad x \in G. \]

In other words, \( x \in G \) and \( y \in Q_G(x) \) if and only if there are \( z \in \mathbb{R}^d \) and \( t \in (0, 1) \) such that

\[ x = ty + (1 - t)z \quad \text{and} \quad x \in P_G(y) \cap P_G(z). \]

Lemma 2.12 states that \( Q_G(x) \) is the largest closed convex subset of \( P_G^{-1}(x) \) whose relative interior contains \( x \).

Let \( 0 < \delta < \epsilon \). As \( P_G^{-1}(x) = \partial \psi_G^\bullet(Sx) \), the convexity and continuity properties of subdifferentials of convex functions yield that

\[ Q_G^\epsilon(x) \subset Q_G^\delta(x), \quad x \in G, \]

\[ \text{graph } Q_G^\epsilon := \{(x, y) \mid x \in G, y \in Q_G^\epsilon(x)\} \text{ is a closed set.} \]

It follows that

\[ \text{graph } Q_G := \{(x, y) \mid x \in G, y \in Q_G(x)\} = \bigcup_{n \geq 1} \text{graph } Q_G^{1/n} \text{ is a } F_\sigma \text{-set,} \]

that is, a countable union of closed sets. In particular, \( \text{graph } Q_G \) is a Borel set in \( \mathbb{R}^{2d} \). This fact is used implicitly in item (c) of Theorem 2.5.

The following theorem is the main result of the paper. We recall that \( \text{supp} \gamma \) stands for the support, the smallest closed set of full measure, of a Borel probability measure \( \gamma \).

**Theorem 2.5.** Let \( S \in \mathcal{S}_m^d \) and \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \). Problems (4) and (6) have solutions and the identical values:

\[ \max_{\gamma \in \Gamma(\nu)} \frac{1}{2} \int S(x, y)d\gamma = \min_{G \in \mathfrak{M}(S)} \int \psi_G d\nu. \]

(8)

For any \( \gamma \in \Gamma(\nu) \) and \( G \in \mathfrak{M}(S) \), the following conditions are equivalent:
(a) \( \gamma \) is an optimal plan for (4) and \( G \) is an optimal set for (6).

(b) (Backward evolution) \( x \in P_G(y) \) for every \( (x, y) \in \text{supp} \gamma \).

(c) (Forward evolution) \( x \in G \) and \( y \in Q_G(x) \), \( \gamma \)-a.s.

Remark 2.6. Theorem A.4 and the construction of the projection multifunction \( P_G \) in (7) yield the equivalence of item (b) to any of the following conditions:

(d) \( \psi_G(y) = S(x, y) - \frac{1}{2} S(x, x) \) and \( x \in G \) for every \( (x, y) \in \text{supp} \gamma \).

(e) \( Sx \in \partial \psi_G(y) \) and \( x \in G \) for every \( (x, y) \in \text{supp} \gamma \).

The proof of Theorem 2.5 is divided into lemmas.

Lemma 2.7. Let \( S \in \mathcal{S}_m^d \), \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \), \( \gamma \in \Gamma(\nu) \), and \( G \in \mathcal{M}(S) \). Then

\[
\frac{1}{2} S(x, x) \leq \psi_G(x) \leq \gamma(\psi_G(y)|x), \quad \gamma \text{-a.s.}, \tag{9}
\]

\[
\int \frac{1}{2} S(x, y) d\gamma = \frac{1}{2} \int S(x, x) d\gamma \leq \int \psi_G d\nu. \tag{10}
\]

Proof. By Theorem A.2, the Fitzpatrick function \( \psi_G \) is convex and \( \psi_G(x) \geq \frac{1}{2} S(x, x) \). The second inequality in (9) follows now from the conditional Jensen inequality and the martingale property of \( \gamma \). The first part of (10) is a consequence of the martingale property of \( \gamma \). The second part of (10) is obtained by integrating (9) over \( \gamma \). \( \square \)

We equip \( \mathcal{P}_2(\mathbb{R}^d) \) with the Wasserstein 2-metric:

\[
W_2(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \sqrt{\int |x - y|^2 d\pi}, \quad \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d),
\]

where \( \Pi(\mu, \nu) \) is the family of Borel probability measures on \( \mathbb{R}^{2d} \) with \( x \)-marginal \( \mu \) and \( y \)-marginal \( \nu \). We recall that \( (\mathcal{P}_2(\mathbb{R}^d), W_2) \) is a Polish space and that \( W_2(\mu_n, \mu) \to 0 \) if and only if \( \mu_n(f) \to \mu(f) \) for every continuous function \( f = f(x) \) on \( \mathbb{R}^d \) with quadratic growth:

\[
|f(x)| \leq K(1 + |x|^2), \quad x \in \mathbb{R}^d,
\]

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where $K = K(f) > 0$ is a constant. A set $A \subset P_2(\mathbb{R}^d)$ is pre-compact under $W_2$ if and only if
\[
\sup_{\mu \in A} \int_{|x| \geq K} |x|^2 d\mu \to 0, \quad K \to \infty. \tag{11}
\]
These results can be found in [1, Chapter 2].

**Lemma 2.8.** If $C$ is a compact set in $(P_2(\mathbb{R}^d), W_2)$, then the set of martingale measures $D = \bigcup_{\nu \in C} \Gamma(\nu)$ is compact in $(P_2(\mathbb{R}^{2d}), W_2)$.

**Proof.** We first show that $D$ is pre-compact. For $\nu \in P_2(\mathbb{R}^d)$, $\gamma \in \Gamma(\nu)$, and a constant $K > 0$, we deduce that
\[
\int |x|^2 1_{\{|x| \geq K\}} d\gamma = \int |\gamma(y|x)|^2 1_{\{|x| \geq K\}} d\gamma \leq \int |y|^2 1_{\{|x| \geq K\}} d\gamma
\]
\[
\leq \int |y|^2 1_{\{|x| \geq K, |y| \geq R\}} d\gamma + \int |y|^2 1_{\{|y| \geq K\}} d\nu
\]
\[
\leq K\gamma(|x| \geq K) + \int |y|^2 1_{\{|y| \geq \sqrt{K}\}} d\nu,
\]
and then that
\[
\frac{1}{2} \int (|x|^2 + |y|^2) 1_{\{|x| + |y| \geq 2K\}} d\gamma \leq \int |x|^2 1_{\{|x| \geq K\}} d\gamma + \int |y|^2 1_{\{|y| \geq K\}} d\nu
\]
\[
\leq \int |y|^2 \left( \frac{1}{K} + 1_{\{|y| \geq \sqrt{K}\}} + 1_{\{|y| \geq K\}} \right) d\nu.
\]
The pre-compactness of $D$ follows now from that of $C$ in view of (11).

To show that $D$ is closed, we take a sequence $(\gamma_n) \subset D$ converging to $\gamma \in P_2(\mathbb{R}^{2d})$ under $W_2$. Let $\nu_n$ and $\nu$ be the $y$-marginals of $\gamma_n$ and $\gamma$. For every continuous function $f = f(y)$ on $\mathbb{R}^d$ with quadratic growth,
\[
\int f(y)d\nu_n = \int f(y)d\gamma_n \to \int f(y)d\gamma = \int f(y)d\nu.
\]
Thus, $\nu_n \to \nu$ in $W_2$. As $C$ is closed, $\nu \in C$. Let $g = g(x)$ be a bounded continuous function on $\mathbb{R}^d$. From the martingale properties of $(\gamma_n)$ we deduce that
\[
\int g(x)(y - x)d\gamma = \lim_{n \to \infty} \int g(x)(y - x)d\gamma_n = 0.
\]
It follows that $\gamma(y|x) = x$ or, equivalently, that $\gamma \in \Gamma(\nu)$. As $\nu \in C$, we obtain that $\gamma \in D$, as required.

**Lemma 2.9** (First-order condition to (4)). Let $S \in S^d_m$, $\nu \in \mathcal{P}_2(\mathbb{R}^d)$, and $\gamma$ be an optimal plan for (4). Then

$$
\int \left( S(x, y) - \frac{1}{2} S(x, x) \right) d\eta \geq \frac{1}{2} S(\eta(y), \eta(y))
$$

for every $\eta \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\text{supp} \eta \subset \text{supp} \gamma$.

**Proof.** We first establish (12) for a Borel probability measure $\eta$ on $\mathbb{R}^d \times \mathbb{R}^d$ having a bounded density $V = V(x, y)$ with respect to $\gamma$. We take any $\theta \in \mathcal{P}_2(\mathbb{R}^d)$ that is singular with respect to $\mu(dx) := \gamma(dx, \mathbb{R}^d)$ and define the product probability measure $\zeta(dx, dy) := \theta(dx)\eta(dy)$ for sufficiently small $\epsilon > 0$, the probability measure $\gamma_\epsilon := \gamma + \epsilon(\zeta - \eta)$ is well defined and has the same $y$-marginal $\nu$ as $\gamma$. We denote $X_\epsilon(x) := \gamma_\epsilon(y|x)$ and observe that the law of $(X_\epsilon, y)$ under $\gamma_\epsilon$ belongs to $\Gamma(\nu)$. From the martingale properties of $\gamma_\epsilon$ and $\gamma$ and the optimality of $\gamma$ we deduce that

$$
\int S(X_\epsilon, X_\epsilon) d\gamma_\epsilon = \int S(X_\epsilon, y) d\gamma_\epsilon \leq \int S(x, y) d\gamma = \int S(x, x) d\gamma.
$$

Let $U(x) := \gamma(V|x)$, $R(x) := \gamma(Vy|x)$, and $A$ be a separating Borel set in $\mathbb{R}^d$ for the singular measures $\mu$ and $\theta$: $\mu(A) = 1 - \theta(A) = 1$. Standard computations based on the Bayes formula show that

$$
X_\epsilon(x) = \gamma_\epsilon(y|x) = 1_{\{x \in A\}} \frac{x - \epsilon R(x)}{1 - \epsilon U(x)} + 1_{\{x \notin A\}} \eta(y), \quad \gamma_\epsilon - a.s.
$$

Since $0 \leq V \leq K$ for some constant $K > 0$, we deduce that $0 \leq U \leq K$ and $|R| \leq K \gamma(|y| |x|)$. Conditional Jensen’s inequality implies that $R$ is square integrable under $\gamma$. It follows that

$$
\int S(X_\epsilon, X_\epsilon) d\gamma_\epsilon = \int \frac{S(x - \epsilon R, x - \epsilon R)}{(1 - \epsilon U)^2} (1 - \epsilon V) d\gamma + \epsilon S(\eta(y), \eta(y))
$$

$$
= \int \frac{S(x - \epsilon R, x - \epsilon R)}{1 - \epsilon U} d\gamma + \epsilon S(\eta(y), \eta(y))
$$

$$
= \int S(x, x) d\gamma + \epsilon (c_1 + S(\eta(y), \eta(y))) + O(\epsilon^2),
$$

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where
\[ c_1 = \int (S(x, x)U - 2S(x, R)) \, d\gamma = \int (S(x, x) - 2S(x, y)) \, V \, d\gamma = \int (S(x, x) - 2S(x, y)) \, d\eta. \]

In view of (13), \( c_1 + S(\eta(y), \eta(y)) \leq 0 \), which is exactly (12).

In the general case, where \( \eta \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) \) and \( \text{supp } \eta \subset \text{supp } \gamma \), we use an approximation argument. Theorem A.1 in [14] yields a sequence \((\eta_n)\) of Borel probability measures on \( \mathbb{R}^{2d} \) having bounded densities with respect to \( \gamma \) and converging to \( \eta \) under \( W_2 \). By what we have already proved,
\[ \int \left( S(x, y) - \frac{1}{2}S(x, x) \right) \, d\eta_n \geq \frac{1}{2} S(\eta_n(y), \eta_n(y)), \quad n \geq 1. \]

Since the integrands are continuous functions with quadratic growth, we can pass to the limit as \( n \to \infty \) and obtain (12).

Lemma 2.10. Let \( S \in \mathbb{S}_m^d \) and \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \). The problems (4) and (6) have solutions and their values are identical.

Proof. By Lemma 2.8, \( \Gamma(\nu) \) is compact in \( (\mathcal{P}_2(\mathbb{R}^{2d}), W_2) \). Since the function \( S = S(x, y) \) is continuous and has quadratic growth, an optimal plan \( \gamma \) exists.

Let \( B(y) \) be the \( y \)-section of \( \text{supp } \gamma \):
\[ B(y) := \{ x \in \mathbb{R}^d \mid (x, y) \in \text{supp } \gamma \}, \quad y \in \mathbb{R}^d, \]
and denote
\[ f(y) := \inf_{x \in B(y)} \left( S(x, y) - \frac{1}{2} S(x, x) \right), \quad y \in \mathbb{R}^d, \]
with the usual convention that \( f(y) = \infty \) if \( B(y) = \emptyset \). Let \( \zeta \) be a probability measure on \( \mathbb{R}^d \) with finite support: \( \text{supp } \zeta = (y_i)_{i=1}^N \). We claim that
\[ \zeta(f) = \sum_{i=1}^N f(y_i) \zeta(\{y_i\}) \geq \frac{1}{2} S(\zeta(y), \zeta(y)). \tag{14} \]
If \( \zeta(f) = \infty \), then (14) holds trivially. Otherwise, for every \( \epsilon > 0 \) there is \( x_i \in B(y_i) \) such that
\[ f(y_i) > S(x_i, y_i) - \frac{1}{2} S(x_i, x_i) - \epsilon, \quad i = 1, \ldots, N. \]
Let $\eta$ be a probability measure on $\mathbb{R}^{2d}$ such that
\[
\eta(\{(x_i, y_i)\}) = \zeta(\{y_i\}), \quad i = 1, \ldots, N.
\]
As $(x_i, y_i) \in \text{supp} \gamma$, we deduce that $\text{supp} \eta \subset \text{supp} \gamma$ and then get (12) from Lemma 2.9. It follows that
\[
\int f(y) d\zeta = \int f(y) d\eta > \int \left( S(x, y) - \frac{1}{2} S(x, x) \right) d\eta - \epsilon
\]
\[
\geq \frac{1}{2} S(\eta(y), \eta(y)) - \epsilon = \frac{1}{2} S(\zeta(y), \zeta(y)) - \epsilon.
\]
As $\epsilon$ is any positive number, we obtain (14).

The minimal property of Fitzpatrick functions from Theorem A.3 yields $G \in \mathcal{M}(S)$ such that $f \geq \psi_G$ or, equivalently, such that
\[
S(x, y) - \frac{1}{2} S(x, x) \geq \psi_G(y), \quad (x, y) \in \text{supp} \gamma.
\]
Accounting for (10), we obtain (8) and the optimality of $G$. \hfill \Box

**Lemma 2.11.** Let $S \in \mathcal{S}_m^d$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. For any $\gamma \in \Gamma(\nu)$ and $G \in \mathcal{M}(S)$, the conditions (a) and (b) of Theorem 2.5 are equivalent.

**Proof.** It is sufficient to show the equivalence of (a) and item (e) of Remark 2.6. By Lemmas 2.7 and 2.10, $\gamma$ and $G$ are optimal if and only if
\[
\frac{1}{2} \int S(x, y) d\gamma = \frac{1}{2} \int S(x, x) d\mu = \int \psi_G(x) d\mu = \int \psi_G(y) d\nu,
\]
where $\mu$ is the $x$-marginal of $\gamma$. Theorem A.2 shows that
\[
\psi^*_G(Sx) \geq \psi_G(x) \geq \frac{1}{2} S(x, x), \quad x \in \mathbb{R}^d,
\]
\[
x \in G \iff \psi_G(x) = \frac{1}{2} S(x, x) \iff \psi^*_G(Sx) = \frac{1}{2} S(x, x).
\]
The optimality of $\gamma$ and $G$ is thus equivalent to the relations:
\[
\mu(G) = 1 \quad \text{and} \quad \int S(x, y) d\gamma = \int (\psi_G(y) + \psi^*_G(Sx)) d\gamma.
\]
By the construction of conjugate functions,
\[
S(x, y) = \langle y, Sx \rangle \leq \psi_G(y) + \psi^*_G(Sx), \quad x, y \in \mathbb{R}^d.
\]
Hence, \( \gamma \) and \( G \) are optimal if and only if
\[
x \in G \text{ and } S(x, y) = \psi_G(y) + \psi_G^*(Sx), \quad \gamma - a.s.,
\]
which is equivalent to item (e) of Remark 2.6, because \( G \) is a closed set and \( \psi_G \) and \( \psi_G^* \) are lower semi-continuous functions.

We denote by \( \text{ri} \ C \) the relative interior of a convex set \( C \), that is, the interior with respect to the Euclidean metric structure restricted to the affine hull of \( C \). If \( C \) is a point: \( C = \{ x_0 \} \), then \( \text{ri} \ C := \{ x_0 \} \).

**Lemma 2.12.** Let \( C \) be a nonempty closed convex set in \( \mathbb{R}^d \) and \( x \in C \). Then
\[
B_C(x) := \{ y \in C \mid x + \epsilon(x - y) \in C \text{ for some } \epsilon > 0 \}
\]
is the largest convex subset of \( C \) whose relative interior contains \( x \). In addition, the set \( B_C(x) \) is closed.

**Proof.** The convexity of \( B_C(x) \) follows from that of \( C \).

Let \( A \) be a convex set. Then \( x \in \text{ri} \ A \) if and only if for every \( y \in A \) there is \( \epsilon > 0 \) such that \( x + \epsilon(x - y) \in A \). This fact shows first that \( x \in \text{ri} \ B_C(x) \) and then that \( B_C(x) \) is the largest convex subset of \( C \) whose relative interior contains \( x \).

Being closed, the set \( C \) contains \( \text{cl} \ B_C(x) \), the closure of \( B_C(x) \). Since \( x \in \text{ri} \ B_C(x) = \text{ri} \ cl \ B_C(x) \), we obtain that \( B_C(x) = \text{cl} \ B_C(x) \).

**Lemma 2.13.** Let \( C \) be a closed convex set in \( \mathbb{R}^d \), \( \mu \in \mathcal{P}_1(\mathbb{R}^d) \) be such that \( \text{supp} \mu \subset C \), and denote \( v := \mu(x) = \int x d\mu \). Then
\[
v \in C \text{ and } \text{supp} \mu \subset B_C(v).
\]

**Proof.** Let \( D := \text{cl conv supp} \mu \), the closed convex hull of the support of \( \mu \). Moving, if necessary, to the affine hull of \( D \) we can assume that \( D \) has a nonempty interior. Clearly, \( v \in D \). If \( v \notin \text{int} D \), then \( v \) belongs to the boundary of \( D \). Fix a normal vector \( u \) to \( D \) at \( v \). We have that
\[
\langle u, v \rangle \geq \langle u, x \rangle, \quad x \in D.
\]
As \( D \) has a nonempty interior, it is not contained in the hyperplane
\[
H := \{ x \in \mathbb{R}^d \mid \langle u, v \rangle = \langle u, x \rangle \}
\].
Since $D = \text{cl conv supp } \mu$, we obtain that
\[ \mu(\{x \mid \langle u, v \rangle \geq \langle u, x \rangle\}) = 1 \text{ and } \mu(\{x \mid \langle u, v \rangle > \langle u, x \rangle\}) > 0 \]
and then arrive to a contradiction:
\[ \langle u, v \rangle > \int \langle u, x \rangle \, d\mu = \langle u, v \rangle. \]
Thus, $v \in \text{ri } D$. As $D \subset C$, Lemma 2.12 shows that $D \subset B_C(v)$. \qed

The following lemma concludes the proof of Theorem 2.5.

**Lemma 2.14.** Let $S \in \mathcal{S}_m^d$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. For $\gamma \in \Gamma(\nu)$ and $G \in \mathcal{M}(S)$, the conditions (b) and (c) of Theorem 2.5 are equivalent.

**Proof.** It is sufficient to show the equivalence of (c) and item (e) of Remark 2.6.

(c) $\Rightarrow$ (e): Being a closed set, $G$ contains the support of $\mu(dx) := \gamma(dx, \mathbb{R}^d)$. Accounting for the martingale property of $\gamma$ and the property (3) of subdifferentials of convex functions, we can choose a regular version of the conditional probability $K(x, dy) := \gamma(dy|x)$ such that
\[ \gamma(y|x) = \int yK(x, dy) = x \text{ and } K(x, \partial \psi_G^*(Sx)) = 1 \text{ for every } x \in G. \]
By Theorem A.2, $G = \{x \mid x \in \partial \psi_G^*(Sx)\}$. Using the notation of Lemma 2.12, we can write $Q_G(x)$ as
\[ Q_G(x) = B_{\partial \psi_G^*(Sx)}(x), \quad x \in G. \]
Lemma 2.13 now yields that $K(x, Q_G(x)) = 1$ for every $x \in G$. The Fubini theorem concludes the argument:
\[ \gamma(\text{graph } Q_G) = \int_G \mu(dx)K(x, Q_G(x)) = \mu(G) = 1. \]
(e) $\Rightarrow$ (c): If $x \in G$, then
\[ y \in Q_G(x) \quad \Rightarrow \quad y \in \partial \psi_G^*(Sx) \quad \iff \quad Sx \in \partial \psi_G(y). \]
It follows that
\[ \text{graph } Q_G \subset A := \{(x, y) \mid x \in G \text{ and } y \in \partial \psi_G^*(Sx)\} \]
and then that $\gamma(A) = 1$. By the closedness of $G$ and the continuity of the subdifferentials of convex functions, $A$ is a closed set. Hence, $\text{supp } \gamma \subset A$, which is exactly (e). \qed
3 Properties of optimal plans

In this section we state some corollaries of Theorem 2.5. We start with a result showing that, for a fixed $G \in \mathcal{M}(S)$, the $F_\sigma$-set

$$\text{graph } Q_G = \{(x, y) \mid x \in G, y \in Q_G(x)\}$$

is pointwise minimal among all Borel sets $B$ in $\mathbb{R}^{2d}$ with the property that $\gamma(B) = 1$ for any $\gamma \in \mathcal{P}_2(\mathbb{R}^{2d})$ such that $\gamma$ and $G$ are solutions to (4) and (6) for some $\nu \in \mathcal{P}_2(\mathbb{R}^d)$.

**Theorem 3.1.** Let $S \in \mathcal{S}^d_m$ and $G \in \mathcal{M}(S)$. Then

$$\text{graph } Q_G = \bigcup_{\gamma \in \Gamma_f(G)} \text{supp } \gamma,$$

where $\Gamma_f(G)$ is the family of probability measures $\gamma$ on $\mathbb{R}^{2d}$ having a finite support and such that $\gamma$ and $G$ are solutions to (4) and (6) for $\nu(dy) = \gamma(R^d, dy)$.

**Proof.** Item (c) of Theorem 2.5 shows that $\text{supp } \gamma \subset \text{graph } Q_G$ for every $\gamma \in \Gamma_f(G)$.

Conversely, let $x \in G$ and $u \in Q_G(x)$. The construction of $Q_G(x)$ yields $v \in Q_G(x)$ and $t \in (0, 1)$ such that $x = tu + (1 - t)v$. Setting

$$\nu\{u\} = \gamma\{(x, u)\} = t, \quad \nu\{v\} = \gamma\{(x, v)\} = 1 - t,$$

we deduce that $\gamma \in \Gamma(\nu)$ and its support set $\{(x, u), (x, v)\}$ is a subset of $\text{graph } Q_G$. By Theorem 2.5, $G$ is optimal for (6). Hence, $\gamma \in \Gamma_f(G)$. \qed

For $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, we write $\mu \prec_{\text{conv}} \nu$ if $\mu$ is dominated by $\nu$ in the convex order: $\mu(f) \leq \nu(f)$ for every positive convex function $f$. By [21, Theorem 2], $\mu \prec_{\text{conv}} \nu$ if and only if $\mu$ is the $x$-marginal of some $\gamma \in \Gamma(\nu)$.

**Theorem 3.2.** Let $S \in \mathcal{S}^d_m$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. The problem

$$\text{maximize } \frac{1}{2} \int S(x, x)d\mu \quad \text{over } \mu \prec_{\text{conv}} \nu,$$

has a solution. Let $\mu \prec_{\text{conv}} \nu$, $G \in \mathcal{M}(S)$, and $\gamma$ belongs to $\Gamma(\nu)$ and has $\mu$ as its $x$-marginal: $\mu(dx) = \gamma(dx, \mathbb{R}^d)$. Then
(a) $\mu$ solves (15) if and only if $\gamma$ is an optimal plan for (4).

(b) $\mu$ solves (15) and $G$ is an optimal set for (6) if and only if

$$\int \psi_G(y)d\nu = \frac{1}{2} \int S(x, x)d\mu.$$

In this case, $\text{supp} \mu \subset G$.

Proof. From the martingale property of $\gamma$ we deduce that

$$\int S(x, y)d\gamma = \int S(x, x)d\gamma = \int S(x, x)d\mu$$

and then get (a). We obtain (b) from the identity above, Theorem 2.5, and the fact that $G$ is closed. \qed

Remark 3.3. Assume that the problem (4) admits a unique optimal plan $\gamma \in \Gamma(\nu)$. According to Theorem 3.2, $\mu(dx) := \gamma(dx, \mathbb{R}^d)$ is the unique solution for (15) and $\gamma$ is the unique martingale coupling between $\mu$ and $\nu$:

$$\rho \in \Gamma(\nu), \rho(dx, \mathbb{R}^d) = \mu(dx) \implies \rho = \gamma.$$  

The latter property is quite special. Usually, probability measures $\mu$ and $\nu$ such that $\mu \prec_{\text{conv}} \nu$ can be coupled by an infinite number of martingale measures.

We now show that an optimal plan $\gamma$ for (4) is a classical optimal $L_2$-coupling between its $Sx$ and $y$ marginals.

Theorem 3.4. Let $S \in S_m^d$, $\nu \in P_2(\mathbb{R}^d)$, $\gamma$ be an optimal plan for (4), and $\mu$ be the $x$-marginal of $\gamma$. Then $\gamma$ is a solution of the (unconstrained) optimal transport problem:

$$\max \quad \int S(x, y)d\pi = \int \langle Sx, y \rangle d\pi \quad \text{over} \quad \pi \in \Pi(\mu, \nu),$$

where $\Pi(\mu, \nu)$ is the family of Borel probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with $x$-marginal $\mu$ and $y$-marginal $\nu$.

Proof. Theorem 2.5 and Remark 2.6 yield $G \in \mathcal{M}(S)$ such that $Sx \in \partial\psi_G(y)$ as soon as $(x, y) \in \text{supp} \gamma$. By the Legendre-Fenchel inequality,

$$\psi_G(y) + \psi_G^*(Sx) \geq \langle y, Sx \rangle = S(x, y), \quad x, y \in \mathbb{R}^d,$$
while by the properties (3) of subdifferentials of convex functions,

\[ \psi_G(y) + \psi_G^*(Sx) = S(x, y), \quad (x, y) \in \text{supp } \gamma. \]

Thus, for every \( \pi \in \Pi(\mu, \nu) \),

\[
\int S(x, y)d\pi \leq \int (\psi_G(y) + \psi_G^*(Sx))d\pi = \int \psi_G(y)d\nu + \int \psi_G^*(Sx)d\mu
\]

\[
= \int (\psi_G(y) + \psi_G^*(Sx))d\gamma = \int S(x, y)d\gamma,
\]

as claimed. \( \square \)

We conclude the section with easy to check sufficient conditions for the uniqueness of the solution to the dual problem (6). The uniqueness of the optimal plan for the primal problem (4) is studied in the follow-up paper [13] and relies on the classification of the singularities of the projection \( P_G \) in [12].

**Theorem 3.5.** Let \( S \in \mathcal{S}^{d}_m \) and \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \). If \( \text{supp } \nu \) is bounded or convex, then the dual problem (6) has a unique solution over \( \text{supp } \nu \) in the sense that

\[ \psi_{\tilde{G}}(y) = \psi_G(y), \quad y \in \text{supp } \nu, \quad \text{and } G \cap \text{supp } \nu = \tilde{G} \cap \text{supp } \nu, \]

for any two optimal sets \( G \) and \( \tilde{G} \).

In particular, if \( \text{supp } \nu \) is convex and there exists an optimal \( G \) contained in \( \text{supp } \nu \), then \( G \) is the unique optimal set. This condition holds trivially if \( \text{supp } \nu = \mathbb{R}^d \).

**Proof.** Consider two optimal sets \( G \) and \( \tilde{G} \) for (6) and let \( \gamma \) be an optimal plan for (4). Item (d) in Remark 2.6 shows that

\[ \psi_G(y) = S(x, y) - \frac{1}{2}S(x, x) = \psi_{\tilde{G}}(y), \quad (x, y) \in \text{supp } \gamma. \]

Denote by \( F \) the projection of \( \text{supp } \gamma \) on the \( y \)-coordinate. While, in the general case, \( F \) may not be closed, we know that \( \text{cl } F = \text{supp } \nu \). From the relation above, it follows that the Fitzpatrick functions \( \psi_G \) and \( \psi_{\tilde{G}} \) coincide and are finite over \( F \).

If \( \text{supp } \nu \) is bounded, the martingale property implies that the \( x \)-projection of \( \text{supp } \gamma \) is bounded as well. A simple compactness argument shows that \( F \) is closed, so \( \text{supp } \nu = F \).
If $C := \text{supp } \nu$ is convex, we have $F \subset C = \text{cl } F$. By restricting to the affine space generated by $C$, we can assume that $C$ has nonempty interior. From $C = \text{cl } F$ we obtain that $\text{int } C = \text{int } \text{conv } F$. The closed convex functions $\psi_G$ and $\tilde{\psi}_G$ are finite on $F$, so they are finite on $\text{conv } F$ and finite and continuous on $\text{int } C$. We know that $\psi_G$ and $\tilde{\psi}_G$ coincide on $F$. Using $\text{cl } F = C$, we obtain that they coincide on $\text{int } C$. Finally, the equality of the closed convex functions $\psi_G$ and $\tilde{\psi}_G$ extends to $\text{cl } \text{int } C = C$.

In both situations, when either $\text{supp } \nu$ is bounded or $\text{supp } \nu$ is convex, it was proved that $\psi_G = \tilde{\psi}_G$ over $\text{supp } \nu$. Now, by the properties of Fitzpatrick functions from Theorem A.2,

$$G \cap \text{supp } \nu = \left\{ x \in \text{supp } \nu \mid \psi_G(x) = \tilde{\psi}_G(x) = \frac{1}{2} S(x,x) \right\} = \tilde{G} \cap \text{supp } \nu.$$

If $\text{supp } \nu$ is convex and there exists an optimal set $G \subset \text{supp } \nu$, then $G = \tilde{G} \cap \text{supp } \nu \subset \tilde{G}$ for any other optimal set $\tilde{G}$. The maximality of $G$ yields that $G = \tilde{G}$. $\square$

4 Linear solutions

The main result of this section, Theorem 4.4, states the necessary and sufficient conditions for a solution to the dual problem (6) to be an affine subset of $\mathbb{R}^d$. In this case, an optimal plan for (4) is unique and has an explicit linear form.

We start with some results from linear algebra. By $I$ we denote the identity matrix and by $V^T$ the transpose of a matrix $V$. Let $A$ be a symmetric $d \times d$ matrix. We write $A > 0$ and say that $A$ is positive definite if $\langle x, Ax \rangle > 0$ for every $x \in \mathbb{R}^d \setminus 0$. We write $A \geq 0$ and say that $A$ is positive semi-definite if $\langle x, Ax \rangle \geq 0$ for every $x \in \mathbb{R}^d$. By $A \leq 0$ we mean that $-A \geq 0$. A similar convention holds for $A < 0$. Notice that $A > 0$ if and only if $A \in \mathbb{S}_d^+$ and $A < 0$ if and only if $A \in \mathbb{S}_d^-$.

**Theorem 4.1.** Let $S \in \mathbb{S}_m^+$ and $\Sigma$ be a symmetric positive definite $d \times d$ matrix. There exist unique symmetric positive semi-definite $d \times d$ matrices $Q$ and $R$ such that

$$\Sigma = Q + R, \quad QSQ \geq 0, \quad RSR \leq 0, \quad QSR = 0. \quad (16)$$
In this case,

\[ \text{rank } Q = m, \quad \text{rank } R = d - m, \quad QS - RSR > 0, \]
\[ Q \Sigma^{-1} Q = Q, \quad R \Sigma^{-1} R = R, \quad Q \Sigma^{-1} R = 0. \]

Proof. The classical diagonalization theorem of linear algebra, [8, Theorem 9, p. 314], yields a \( d \times d \) matrix \( V \) of full rank such that

\[ V^T S V = \Lambda, \quad V^T \Sigma^{-1} V = I, \]

where \( \Lambda \) is a diagonal matrix: \( \Lambda_{ij} = \delta_{ij} \lambda_i \), whose first \( m \) diagonal elements are strictly positive and the remaining \( d - m \) diagonal elements are strictly negative.

Observe now that the symmetric positive semi-definite matrices \( Q \) and \( R \) satisfy (16) if and only if

\[ Q = VAV^T, \quad R = VBV^T, \]

where \( A \) and \( B \) are positive semi-definite matrices such that

\[ I = A + B, \quad A \Lambda A \geq 0, \quad B \Lambda B \leq 0, \quad A \Lambda B = 0. \]

We claim that the only such \( A \) and \( B \) are diagonal and given by

\[ A_{ij} = \delta_{ij} \mathbb{1}_{\{i \leq m\}}, \quad B_{ij} = \delta_{ij} \mathbb{1}_{\{i > m\}}, \quad i, j \in \{1, \ldots, d\}. \]

Checking that the above matrices \( A \) and \( B \) are solutions is immediate. The uniqueness is verified as follows.

From \( A \Lambda B = 0 \) and \( A + B = I \) we obtain that \( \Lambda A = A \Lambda A \) and \( \Lambda B = B \Lambda B \). In particular, the matrix \( \Lambda A \) is symmetric:

\[ \lambda_i A_{ij} = \lambda_j A_{ji}, \quad i, j \in \{1, \ldots, d\}. \]

Because \( A \) is symmetric and \( \lambda_i > 0 \) for \( i \leq m \) and \( \lambda_i < 0 \) for \( i > m \), we deduce that

\[ A_{ij} = A_{ji} = 0, \quad i \leq m < j. \]

Since \( \Lambda A = A \Lambda A \geq 0 \), we have that

\[ 0 \leq \sum_{ij} \lambda_i A_{ij} x_i x_j = \sum_i \lambda_i A_{ii} x_i^2 + \sum_{i<j} (\lambda_i + \lambda_j) A_{ij} x_i x_j, \quad x \in \mathbb{R}^d. \]
Recalling that $A \geq 0$, taking distinct $k, l \in \{m+1, \ldots, d\}$, and choosing $x_i = \delta_{ik}$ and $x_i = \delta_{ik} + \delta_{il}$ we obtain that

$$A_{kl} = 0, \quad k, l > m.$$  

Thus the matrix $A$ has possible nonzero entries $A_{ij}$ only for $i, j \leq m$. Using $A \Lambda B = B \Lambda A \leq 0$ and $B \geq 0$ we go over identical arguments to obtain that the matrix $B$ has possible nonzero entries $B_{ij}$ only for $i, j > m$. The uniqueness follows now from $A + B = I$.

We have shown that symmetric positive semi-definite matrices $Q$ and $R$ satisfying (16) exist and are unique. The remaining properties of $Q$ and $R$ follow from their counterparts for $A$ and $B$:

$$\text{rank } A = m, \quad \text{rank } B = d - m, \quad A \Lambda A - B \Lambda B > 0, \quad AIA = A, \quad BIB = B, \quad AIB = 0.$$

We recall that a $d \times d$ matrix $P$ is called idempotent if $P^2 = P$.

**Theorem 4.2.** Let $S \in \mathcal{S}_m^d$, $\Sigma$ be a symmetric positive definite $d \times d$ matrix, and $Q$ and $R$ be the symmetric positive semi-definite matrices satisfying (16). Then $P := Q \Sigma^{-1}$ is the unique idempotent $d \times d$ matrix such that

- the matrices $P \Sigma$ and $S \Sigma$ are symmetric,
- $P \Sigma \geq 0$, \quad $(I - P) \Sigma \geq 0$, \quad $S \Sigma \geq 0$, \quad $S(I - P) \leq 0$. \quad (17)

In this case,

$$SP - S(I - P) = S(2P - I) > 0.$$

**Proof.** We have that $P \Sigma = Q \geq 0$, $(I - P) \Sigma = R \geq 0$, and

$$P^TSP = \Sigma^{-1}RSQ\Sigma^{-1} = 0,$$

$$SP = P^TSP = \Sigma^{-1}QS\Sigma^{-1} \geq 0,$$

$$S(I - P) = (I - P)^T S(I - P) = \Sigma^{-1} RSR\Sigma^{-1} \leq 0. \quad (18)$$

By Theorem 4.1, $Q \Sigma^{-1}Q = Q$, so

$$P^2 = Q \Sigma^{-1}Q \Sigma^{-1} = Q \Sigma^{-1} = P.$$
Thus, \( P \) is an idempotent matrix solving (17). Moreover, by Theorem 4.1,

\[
SP - S(I - P) = \Sigma^{-1}(QSQ - RSR)\Sigma^{-1} > 0.
\]

Conversely, if \( P' \) is an idempotent matrix solving (17), then the relations in (18) (applied in the reverse order) show that \( Q' := P'\Sigma \) and \( R' := (I - P')\Sigma \) are symmetric positive semi-definite matrices satisfying (16). The uniqueness part of Theorem 4.1 yields that \( Q' = Q \). Hence, \( P = P' \).

We conclude the introductory part of the section with a description of all affine maximal strictly (in the sense of (19)) \( S \)-monotone sets.

**Theorem 4.3.** Let \( S \in \mathcal{S}_m^d \). The following conditions are equivalent:

(a) \( G \) is an affine subspace of \( \mathbb{R}^d \), \( G \in \mathfrak{M}(S) \), and

\[
S(x - y, x - y) > 0, \quad x, y \in G, \ x \neq y.
\] (19)

(b) \( G = \{ x_0 + P(x - x_0) \mid x \in \mathbb{R}^d \} \), where \( x_0 \in \mathbb{R}^d \) and \( P \) is a \( d \times d \) idempotent matrix such that the matrix \( SP \) is symmetric and

\[
SP \geq 0, \quad S(I - P) \leq 0, \quad S(2P - I) > 0.
\] (20)

The projection on \( G \) in the \( S \)-space has the form:

\[
P_G(y) := \arg \min_{x \in G} S(y - x, y - x) = x_0 + P(y - x_0), \quad y \in \mathbb{R}^d.
\]

**Proof.** Without restriction of generality we can assume that \( G \) is a linear subspace, that is, it contains 0. We then take \( x_0 = 0 \).

(a) \( \implies \) (b): Standard arguments show that for every \( y \in \mathbb{R}^d \) the function \( x \to S(y - x, y - x) \) attains the minimum on \( G \) at a unique \( P_G(y) \) such that

\[
S(y - P_G(y), x) = 0, \quad x \in G.
\] (21)

We first observe that \( P_G(y) = y \) for \( y \in G \). Then, since \( G \) is a linear subspace, we deduce that \( P_G \) is a linear function mapping \( \mathbb{R}^d \) onto \( G \):

\[
P_G(y) = Py, \quad y \in \mathbb{R}^d,
\]

for a unique \( d \times d \)-matrix \( P \). As

\[
P^2 y = P_G(P_G(y)) = P_G(y) = Py, \quad y \in \mathbb{R}^d.
\]
$P$ is an idempotent matrix. Since

$$G = \text{range } P_G := \{ P_G(y) \mid y \in \mathbb{R}^d \} = \{ Py \mid y \in \mathbb{R}^d \},$$

we can write (21) as

$$S(y - Py, Px) = \langle (I - P)y, SPx \rangle = 0, \quad x, y \in \mathbb{R}^d,$$

or, equivalently, as

$$0 = (I - P)^T SP = SP - P^T SP.$$

In particular, $SP$ is a symmetric matrix. As $\text{range } P = G$, we deduce from (19) that $SP = P^T SP \geq 0$. Since $G \in \mathcal{M}(S)$, we obtain that

$$S(y - Py, y - Py) = \min_{x \in G} S(y - x, y - x) < 0, \quad y \in \mathbb{R}^d \setminus G.$$

As $y = Py$, $y \in G$, and $SP = P^T S = P^T SP$, we deduce that

$$0 \geq (I - P)^T S(I - P) = S(I - P).$$

Accounting for (19) we also obtain that

$$0 < P^T SP - (I - P)^T S(I - P) = SP - S(I - P) = S(2P - I).$$

(b) $\implies$ (a): Recall that $x_0 = 0$ and thus,

$$G := \text{range } P = \{ Py \mid y \in \mathbb{R}^d \}.$$

To finish the proof of the theorem, we have to show that $G \in \mathcal{M}(S)$ and that (19) holds. If $x \in G$, then $x = (2P - I)x$. Since the matrix $U := S(2P - I)$ is positive definite, we obtain that

$$S(x, x) = S(x, (2P - I)x) = \langle x, Ux \rangle > 0, \quad x \in G \setminus 0.$$

Hence, $G$ is an $S$-monotone set satisfying (19).

As $(2P - I)(I - P) = -(I - P)$, we obtain that

$$(I - P)^T U(I - P) = -(I - P)^T S(I - P).$$

If $y \notin G$, then $z := y - Py = (I - P)y \neq 0$. It follows that

$$S(z, z) = \langle (I - P)y, S(I - P)y \rangle = -\langle (I - P)y, U(I - P)y \rangle = -\langle z, Uz \rangle < 0.$$

Since $Py \in G$, this proves the maximality of $G$. 

\[\square\]
For simplicity of notation, in Theorems 4.4 and 4.5 we use a probabilistic setup. We start with a $d$-dimensional random variable $Y$ on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ having a finite second moment: $Y \in L_2(\mathbb{R}^d)$. We denote $\nu := \text{Law}(Y)$, the law of $Y$. Let $X \in L_2(\mathbb{R}^d)$. Clearly, $\text{Law}(X, Y) \in \Gamma(\nu)$ if and only if $X = \mathbb{E}(Y | X)$. As usual, we interpret all relations between random variables in the $\mathbb{P}$-a.s. sense.

**Theorem 4.4.** Let $S \in S_m^d$, $Y \in L_2(\mathbb{R}^d)$, assume that the covariance matrix of $Y$ is positive definite:

$$\Sigma := \mathbb{E}((Y - \mathbb{E}(Y))(Y - \mathbb{E}(Y))^T) > 0,$$

and denote $\nu := \text{Law}(Y)$. Let $P$ be the unique idempotent $d \times d$ matrix satisfying (17). The following conditions are equivalent:

(a) An optimal set $G$ for (6) is an affine subspace of $\mathbb{R}^d$.

(b) The random variable $X := \mathbb{E}(Y) + P(Y - \mathbb{E}(Y))$ has the martingale property: $\mathbb{E}(Y | X) = X$.

In this case, the law of $(X, Y)$ is the unique optimal plan for (4) and

$$G := \{\mathbb{E}(Y) + P(x - \mathbb{E}(Y)) \mid x \in \mathbb{R}^d\}$$

(22)

is the unique affine subspace of $\mathbb{R}^d$ which is an optimal set for (6).

If $G = \text{supp} \mu$ for $\mu := \text{Law}(X)$, then $G$ is the unique optimal set.

**Proof.** (a) $\implies$ (b): Let us show (19). If this condition fails, then there are distinct $x_0, x_1 \in G$ such that $S(x_1 - x_0, x_1 - x_0) = 0$. As $G$ is an affine subspace,

$$x(t) := x_0 + t(x_1 - x_0) \in G, \quad t \in \mathbb{R},$$

and we obtain the lower bound for the Fitzpatrick function $\psi_G$:

$$\psi_G(y) = \sup_{x \in G} \left( S(x, y) - \frac{1}{2} S(x, x) \right) \geq \sup_{t \in \mathbb{R}} \left( S(x(t), y) - \frac{1}{2} S(x(t), x(t)) \right)$$

$$= S(x_0, y) - \frac{1}{2} S(x_0, x_0) + \sup_{t \in \mathbb{R}} (tS(y - x_0, x_1 - x_0)).$$

It follows that the domain of $\psi_G$ is contained in the hyperplane

$$H := \{y \in \mathbb{R}^d \mid S(y - x_0, x_1 - x_0) = 0\}$$

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of dimension $d - 1$. As $\mathbb{E} (\psi_G(Y)) = \int \psi_G(y) d\nu < \infty$, we deduce that $Y \in H$. In particular, the random variables $(Y^n)_{n=1,\ldots,d}$ are linearly dependent, in contradiction with the assumption that their covariance matrix $\Sigma > 0$.

Given (19), Theorem 4.3 states that

$$G = \left\{ x_0 + \tilde{P}(x - x_0) \mid x \in \mathbb{R}^d \right\}$$

for the idempotent matrix $\tilde{P}$ satisfying (20) and some $x_0 \in \mathbb{R}^d$. It also shows that the projection on $G$ in the $S$-space has the form:

$$P_G(y) = x_0 + \tilde{P}(y - x_0), \quad y \in \mathbb{R}^d.$$

By Theorem 2.5, an optimal plan for (4) exists. Moreover, as $G$ is an optimal set for (6), every optimal plan $\gamma$ is supported on the graph $\{(P_G(y), y) \mid y \in \mathbb{R}^d\}$. Since the projection $P_G$ is single-valued, such $\gamma$ is unique and given by the joint law of $(X,Y)$, where

$$X := P_G(Y) = x_0 + \tilde{P}(Y - x_0).$$

In particular, $X = \mathbb{E} (Y \mid X)$ and

$$\mathbb{E} (Y) = \mathbb{E} (X) = x_0 + \tilde{P}(\mathbb{E} (Y) - x_0).$$

It follows that

$$G = \left\{ x_0 + \tilde{P}(x - x_0) \mid x \in \mathbb{R}^d \right\} = \left\{ \mathbb{E} (Y) + \tilde{P}(x - \mathbb{E} (Y)) \mid x \in \mathbb{R}^d \right\}.$$ 

Thus, we can take $x_0 = \mathbb{E} (Y)$.

As $X = \mathbb{E} (Y \mid X)$, we have that

$$0 = \mathbb{E} \left( (Y - X)(X - \mathbb{E} (X))^T \right) = (I - \tilde{P}) \Sigma \tilde{P}^T = \Sigma \tilde{P}^T - \tilde{P} \Sigma \tilde{P}^T$$

$$= (I - \tilde{P}) \Sigma - (I - \tilde{P}) \Sigma (I - \tilde{P})^T.$$

It follows that $\Sigma \tilde{P}^T$ and $(I - \tilde{P}) \Sigma$ are symmetric positive semi-definite:

$$\Sigma \tilde{P}^T = \tilde{P} \Sigma \tilde{P}^T = \mathbb{E} \left( (X - \mathbb{E} (X))(X - \mathbb{E} (X))^T \right) \geq 0,$$

$$(I - \tilde{P}) \Sigma = (I - \tilde{P}) \Sigma (I - \tilde{P})^T = \mathbb{E} \left( (Y - X)(Y - X)^T \right) \geq 0.$$

Thus, $\tilde{P}$ is a solution of (17). Theorem 4.2 shows that $P = \tilde{P}$. Hence, $G$ is given by (22).
(b) \implies (a): By Theorems 4.2 and 4.3, the set $G$ in (22) belongs to $\mathcal{M}(S)$ and $X = P_{G}(Y)$. Theorem 2.5 shows that $G$ is an optimal set for (6) and $\gamma := \text{Law}(X,Y)$ is the unique optimal plan for (4).

If $\tilde{G}$ is another optimal set (not necessarily affine), then item (c) of Theorem 2.5 yields that
$$\text{supp } \mu \subset G \cap \tilde{G}.$$ If $\text{supp } \mu = G$, then $G \subset \tilde{G}$ and the maximality of $G$ implies that $G = \tilde{G}$.

Assume the setup of Theorem 4.4 and that $E(Y) = 0$. Item (b) of Theorem 4.4 can be equivalently stated as
$$E\left((I - P)Y \mid PY\right) = 0.$$ Since $(I - P)\Sigma P^T = 0$, item (b) holds if
$$A\Sigma B^T = 0 \implies E(AY \mid BY) = 0,$$ for all $d \times d$ matrices $A$ and $B$. This is the case, for instance, if $Y$ has a Gaussian or, more generally, elliptically contoured distribution with mean zero and covariance matrix $\Sigma$.

**Theorem 4.5.** Let $S \in S^d_m$ and $Y$ be a $d$-dimensional Gaussian random variable with mean zero and the covariance matrix $\Sigma > 0$. Let $P$ be the unique idempotent $d \times d$ matrix satisfying (17). Then
$$X = PY, \quad Z = (I - P)Y,$$ are the unique independent $d$-dimensional Gaussian random variables with mean zero such that
$$Y = X + Z, \quad S(X,X) \geq 0, \quad S(Z,Z) \leq 0, \quad S(X,Z) = 0.$$ The law of $(X,Y)$ is the unique optimal plan for (4) and
$$\text{range } P := \{Px \mid x \in \mathbb{R}^d\}$$ is the unique optimal set for (6), where $\nu := \text{Law}(Y)$. 

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Proof. Clearly, $X$ and $Z$ are $d$-dimensional Gaussian random variables with mean zero. Their covariance matrices are given by
\[
\begin{align*}
\mathbb{E}(XX^T) &= P\mathbb{E}(YY^T)P^T = P\Sigma P^T = P\Sigma, \\
\mathbb{E}(ZZ^T) &= (I - P)\Sigma(I - P)^T = (I - P)\Sigma, \\
\mathbb{E}(XZ^T) &= P\Sigma(I - P)^T = 0.
\end{align*}
\]

The last identity implies that $X$ and $Z$ are independent random variables. The relations (23) readily follow from the properties (17) of the idempotent matrix $P$.

Let $X'$ and $Z'$ be independent $d$-dimensional Gaussian random variables with mean zero, the covariance matrices $Q'$ and $R'$, respectively, and such that
\[
\begin{align*}
Y &= X' + Z', \\
S(X', X') &\geq 0, \quad S(Z', Z') \leq 0, \quad S(X', Z') = 0.
\end{align*}
\]

As $X'$ and $Z'$ are Gaussian random variables, their laws are supported by the ranges of the covariance matrices. Accounting for the independence of $X'$ and $Z'$ we deduce that
\[
Q' + R' = \Sigma, \\
S(x, x) &\geq 0, \quad S(z, z) \leq 0, \quad S(x, z) = 0, \quad x \in \text{range } Q', \quad z \in \text{range } R',
\]
and then that
\[
Q'SQ' \geq 0, \quad R'SR' \leq 0, \quad Q'SR' = 0.
\]

Theorem 4.2 shows that $P = Q'\Sigma^{-1}$. Then $Q' = P\Sigma$ and $R' = (I - P)\Sigma$ are also the covariance matrices of $X$ and $Z$, respectively. It follows that $\text{Law}(X', Z') = \text{Law}(X, Z)$, that
\[
\text{Law}(X', Y) = \text{Law}(X, Y) = \text{Law}(PY, Y),
\]
and then that $X' = PY = X$ and $Z' = Y - X' = Y - X = Z$.

Finally, Theorem 4.4 yields the optimality and uniqueness properties of $\gamma := \text{Law}(X, Y)$ and $G := \text{range } P$. 

\[\square\]
A Fitzpatrick functions in the $S$-space

For $S \in S^d_m$, the family of symmetric $d \times d$-matrices of full rank with $m$ positive eigenvalues, we recall the notation

$$S(x, y) := \langle x, Sy \rangle = \langle Sx, y \rangle, \quad x, y \in \mathbb{R}^d,$$

for the bilinear form and $\mathcal{M}(S)$ for the family of maximal $S$-monotone sets. Clearly, $S^{-1}$, the inverse matrix to $S$, belongs to $S^d_m$.

For $S \in S^2_m$ from Example 2.3, many results of this appendix can be found in [7] and [17]. The case of general symmetric $S$ has been studied in [20] and [16].

**Theorem A.1.** Let $S \in S^d_m$ and $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ be a closed convex function such that

$$\min(f(x), f^*(Sx)) \geq \frac{1}{2}S(x, x), \quad x \in \mathbb{R}^d. \quad (24)$$

Then the set $G := \{x \in \mathbb{R}^d \mid Sx \in \partial f(x)\}$ belongs to $\mathcal{M}(S)$ and has equivalent descriptions:

$$G = \left\{ x \in \mathbb{R}^d \mid f(x) = \frac{1}{2}S(x, x) \right\} = \left\{ x \in \mathbb{R}^d \mid f^*(Sx) = \frac{1}{2}S(x, x) \right\}. \quad (25)$$

**Proof.** By the properties (3) of subdifferentials of convex functions,

$$Sx \in \partial f(x) \iff x \in \partial f^*(Sx) \iff f(x) + f^*(Sx) = S(x, x).$$

The latter representation and (24) imply that

$$G = \left\{ x \in \mathbb{R}^d \mid f(x) = f^*(Sx) = \frac{1}{2}S(x, x) \right\}.$$

Let $u \in \mathbb{R}^d$. If $f(x) = \frac{1}{2}S(x, x)$, then inequality (24) yields that

$$\lim_{t \downarrow 0} \frac{1}{t} (f(x + tu) - f(x)) \geq \lim_{t \downarrow 0} \frac{1}{2t} (S(x + tu, x + tu) - S(x, x)) \quad = S(x, u) = \langle Sx, u \rangle.$$

It follows that $Sx \in \partial f(x)$, proving the first equality in (25).
Similarly, if $f^*(Sx) = \frac{1}{2}S(x, x)$, then
\[
\lim_{t \downarrow 0} \frac{1}{t} \left( f^*(Sx + tu) - f^*(Sx) \right) \geq \lim_{t \downarrow 0} \frac{1}{2t} \left( S(x + tS^{-1}u, x + tS^{-1}u) - S(x, x) \right) = S(x, S^{-1}u) = \langle x, u \rangle.
\]
It follows that $x \in \partial f^*(Sx)$ or equivalently, that $Sx \in \partial f(x)$, proving the second equality in (25).

If $x, y \in G$, then $(x, Sx)$ and $(y, Sy)$ belong to the graph of $\partial f$, which is a classical monotone set in $\mathbb{R}^{2d}$:
\[
S(x - y, x - y) = \langle x - y, Sx - Sy \rangle \geq 0.
\]
Hence, $G$ is $S$-monotone.

To show that $G$ is maximal, we assume first that $S$ is an orthogonal matrix:
\[
S = S^{-1}.
\]
In this case, condition (24) becomes symmetric with respect to $f$ and $f^*$:
\[
\max (f(x), f^*(x)) \geq \frac{1}{2}S(x, x), \quad x \in \mathbb{R}^d.
\]
(26)
For every $v \in \mathbb{R}^d$, the Moreau decomposition from [19, Theorem 31.5, p. 338] yields unique $x \in \text{dom} \partial f$ and $y \in \partial f(x)$ such that $v = x + y$. Taking $u \in \mathbb{R}^d \setminus G$ and setting $v = u + Su$ we obtain that
\[
u + Su = x + y.
\]
The orthogonality of $S$ yields that
\[
Sx + Sy = Su + S^2u = Su + u = x + y.
\]
It follows that $x - Sy = Sx - y$ and
\[
|x - Sy|^2 = |Sx - y|^2 = \langle x - Sy, Sx - y \rangle.
\]
On the other hand, from (26), the orthogonality of $S$, and the fact that $y \in \partial f(x)$ we deduce that
\[
\frac{1}{2} \langle x - Sy, Sx - y \rangle = \frac{1}{2} (S(x, x) + S(y, y) - \langle x, y \rangle - \langle Sx, Sy \rangle)
\]
\[
= \frac{1}{2} (S(x, x) + S(y, y)) - \langle x, y \rangle
\]
\[
\leq f(x) + f^*(y) - \langle x, y \rangle = 0.
\]
It follows that $Sx = y \in \partial f(x)$ and then that $x \in G$. Since $u + Su = x + y = x + Sx$, we have that $x - u = Su - Sx$. It follows that

$$S(x - u, x - u) = \langle x - u, Sx - Su \rangle = -|x - u|^2 < 0,$$

proving the maximality of the $S$-monotone set $G$.

In the general case, we decompose the symmetric matrix $S$ as

$$S = V^T U V,$$

where $V$ is a $d \times d$-matrix of full rank and $U$ is symmetric and orthogonal. The law of inertia for quadratic forms, [8, Theorem 1, p. 297], states that $U \in S^d_m$. We can actually take $U$ to be of the canonical form of Example 2.4. It is easy to see that

$$S(x, x) = U(Vx, Vx), \quad x \in \mathbb{R}^d,$$

and

$$G \in \mathcal{M}(S) \iff F := VG = \{x \mid V^{-1}x \in G\} \in \mathcal{M}(U).$$

We define the closed convex function

$$g(x) := f(V^{-1}x), \quad x \in \mathbb{R}^d,$$

and deduce from (25) that

$$F = \left\{ x \mid f(V^{-1}x) = \frac{1}{2} S(V^{-1}x, V^{-1}x) \right\} = \left\{ x \mid g(x) = \frac{1}{2} U(x, x) \right\}.$$

In view of (24) we have that

$$g(x) \geq \frac{1}{2} S(V^{-1}x, V^{-1}x) = \frac{1}{2} U(x, x),$$

$$g^*(y) = \sup_{x \in \mathbb{R}^d} \langle (Vx, y) - g(Vx) \rangle = \sup_{x \in \mathbb{R}^d} \langle (x, V^T y) - f(x) \rangle = f^*(V^T y),$$

$$g^*(Ux) = f^*(V^T Ux) = f^*(SV^{-1}x) \geq \frac{1}{2} S(V^{-1}x, V^{-1}x) = \frac{1}{2} U(x, x).$$

Thus, $F \in \mathcal{M}(U)$ by what has been already proved.

Let $G \in \mathcal{M}(S)$. We recall that the Fitzpatrick function $\psi_G$ is defined as

$$\psi_G(y) = \sup_{x \in G} \left( S(x, y) - \frac{1}{2} S(x, x) \right), \quad y \in \mathbb{R}^d.$$
**Theorem A.2.** Let $S \in S_m^d$ and $G \in \mathcal{M}(S)$. The Fitzpatrick function $\psi_G$ is a closed convex function on $\mathbb{R}^d$ taking values in $\mathbb{R} \cup \{+\infty\}$ such that

$$\psi^*_G(Sx) \geq \psi_G(x) \geq \frac{1}{2}S(x,x), \quad x \in \mathbb{R}^d. \quad (27)$$

We have that

$$x \in G \iff Sx \in \partial \psi_G(x) \iff x \in \partial \psi^*_G(Sx) \iff \psi_G(x) = \frac{1}{2}S(x,x) \iff \psi^*_G(Sx) = \frac{1}{2}S(x,x). \quad (28)$$

**Proof.** Being an upper envelope of a family of linear functions, $\psi_G$ is a closed convex function taking values in $\mathbb{R} \cup \{+\infty\}$. We have that

$$S(x,x) - 2\psi_G(x) = \phi_G(x) := \inf_{y \in G} S(x - y, x - y), \quad x \in \mathbb{R}^d. \quad (27)$$

As $G$ is $S$-monotone, $\psi_G(x) = \frac{1}{2}S(x,x), \quad x \in G$. The maximal $S$-monotonicity of $G$ yields that $\psi_G(x) > \frac{1}{2}S(x,x), \quad x \notin G$, as, otherwise, $G \cup \{x\}$ is an $S$-monotone set. Therefore, $\psi_G(x) \geq \frac{1}{2}S(x,x), \quad x \in \mathbb{R}^d$, and $x \in G$ if and only if $\psi_G(x) = \frac{1}{2}S(x,x)$. We now have

$$\psi^*_G(Sy) = \sup_{x \in \mathbb{R}^d} (\langle x, Sy \rangle - \psi_G(x)) \geq \sup_{x \in G} \left( S(x,y) - \frac{1}{2}S(x,x) \right)$$

$$= \psi_G(y) \geq \frac{1}{2}S(y,y), \quad y \in \mathbb{R}^d,$$

proving (27).

The second equivalence in (28) holds by the properties (3) of subdifferentials of convex functions. Theorem A.1 yields the other equivalences, completing the proof.

For a function $f$ taking values in $\mathbb{R} \cup \{+\infty\}$, we denote by $\text{conv} f$ its convex hull, that is the largest convex function smaller than $f$, and by $\text{cl conv} f$ its closed convex hull:

$$\text{cl conv} f(x) = \lim \inf_{y \to x} \text{conv} f(y) := \lim_{\varepsilon \downarrow 0} \inf_{|y - x| < \varepsilon} \text{conv} f(y).$$

We denote by $\mathcal{P}_f(\mathbb{R}^d)$ the family of probability measures on $\mathbb{R}^d$ with finite support.
Theorem A.3. Let $S \in S^d_m$. For a function $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, the following conditions are equivalent:

(a) For every $\mu \in \mathcal{P}_f (\mathbb{R}^d)$,
$$\mu(f) := \int f d\mu \geq \frac{1}{2} S(\mu(x), \mu(x)).$$

(b) $\text{cl conv } f(x) \geq \frac{1}{2} S(x, x), x \in \mathbb{R}^d$.

(c) There is $G \in \mathfrak{M}(S)$ such that $f \geq \psi_G$.

Proof. (c) $\implies$ (a): By Theorem A.2, $\psi_G$ is convex and $\psi_G(x) \geq \frac{1}{2} S(x, x), x \in \mathbb{R}^d$. For $\mu \in \mathcal{P}_f (\mathbb{R}^d)$, the convexity of $\psi_G$ yields that
$$\mu(f) \geq \mu(\psi_G) \geq \frac{1}{2} S(\mu(x), \mu(x)).$$

(a) $\implies$ (b): We recall, [19, Theorem 5.6, p. 37], that
$$\text{conv } f(y) = \inf \{\mu(f) \mid \mu \in \mathcal{P}_f (\mathbb{R}^d), \mu(x) = y\}, \ y \in \mathbb{R}^d.$$ It follows that $\text{conv } f(x) \geq \frac{1}{2} S(x, x), x \in \mathbb{R}^d$. Finally,
$$\text{cl conv } f(x) = \liminf_{y \to x} \text{conv } f(y) \geq \frac{1}{2} \liminf_{y \to x} S(y, y) = \frac{1}{2} S(x, x).$$

(b) $\implies$ (c): Let $\Psi$ be the family of closed convex functions $g = g(x)$ on $\mathbb{R}^d$ such that $g(x) \geq \frac{1}{2} S(x, x)$. We call $h \in \Psi$ minimal if there is no $g \in \Psi$ such that $g \leq h$ and $g \neq h$.

Claim 1. For every $g \in \Psi$, there is a minimal $h \in \Psi$ such that $g \geq h$.

Proof. For $h \in \Psi$, we write
$$\Psi(h) := \{\tilde{h} \in \Psi \mid \tilde{h} \leq h\}.$$ Clearly, $\text{dom } h \subset \text{dom } \tilde{h}, \tilde{h} \in \Psi(h)$. By moving, if necessary, to a smaller element $g \in \Psi$, we can assume from the start that the domain of every element of $\Psi(g)$ has the same affine hull:
$$L := \text{aff dom } g = \text{aff dom } h, \ h \in \Psi(g).$$
Let \( \mu \) be a Borel probability measure on \( L \) having a strictly positive density with respect to the Lebesgue measure on \( L \). For \( h \in \Psi(g) \), we denote

\[
\alpha(h) := \sup_{\tilde{h} \in \Psi(h)} \left( \mu \left( \text{dom} \tilde{h} \setminus \text{dom} h \right) \right) = \sup_{\tilde{h} \in \Psi(h)} \left( \mu(\text{dom} \tilde{h}) - \mu(\text{dom} h) \right).
\]

We define a sequence \((h_n)\) in \( \Psi(g) \) such that \( h_1 = g \), \( h_{n+1} \in \Psi(h_n) \), and \( \mu(\text{dom} h_{n+1} \setminus \text{dom} h_n) \geq \alpha(h_n)/2 \). We have that

\[
\alpha(h_{n+1}) \leq \alpha(h_n) - \mu(\text{dom} h_{n+1} \setminus \text{dom} h_n) \leq \frac{1}{2} \alpha(h_n) \leq \left( \frac{1}{2} \right)^n \alpha(g) \to 0.
\]

Being bounded below by \( \frac{1}{2}S(x,x) \), the functions \((h_n)\) converge pointwise to a convex (not necessarily closed) function \( \tilde{h} \). Clearly, the closure \( h \) of \( \tilde{h} \) belongs to \( \Psi(g) \) and has the property: \( \alpha(h) = 0 \).

By the above arguments, we can assume from the start that \( \alpha(g) = 0 \) or, equivalently, that

\[
D := \text{ri dom}(g) = \text{ri dom} h, \quad h \in \Psi(g).
\]

We take a Borel probability measure \( \nu \) on \( D \) having a strictly positive density with respect to the Lebesgue measure on \( D \) and such that

\[
\int (g(x) - \frac{1}{2}S(x,x))d\nu < \infty.
\]

For \( h \in \Psi(g) \), we denote

\[
\beta(h) := \sup_{\tilde{h} \in \Psi(h)} \nu \left( h - \tilde{h} \right).
\]

We define a sequence \((h_n)\) in \( \Psi(g) \) such that \( h_1 = g \), \( h_{n+1} \in \Psi(h_n) \), and \( \nu(h_n - h_{n+1}) \geq \beta(h_n)/2 \). We have that

\[
\beta(h_{n+1}) \leq \beta(h_n) - \nu(h_n - h_{n+1}) \leq \frac{1}{2} \beta(h_n) \leq \left( \frac{1}{2} \right)^n \beta(g) \to 0.
\]

The functions \((h_n)\) converge pointwise on the relatively open \( D \) to a finite convex function \( h \) on \( D \). We extend \( h \) by semi-continuity to \( \text{cl} D \) and set its values to \( \infty \) outside of \( \text{cl} D \). We obtain a closed convex function. Clearly, \( h \in \Psi(g) \) and \( \beta(h) = 0 \). If \( \tilde{h} \in \Psi(h) \), then \( \tilde{h} = h \) on \( D \), the common relative interior of their domains. Being closed convex functions, \( h \) and \( \tilde{h} \) are identical. Hence, \( h \) is a minimal element of \( \Psi(g) \).
Claim 2. If $h$ is a minimal element of $\Psi$, then

$$h^*(Sx) \geq \frac{1}{2}S(x,x), \quad x \in \mathbb{R}^d.$$ 

Proof. Assume to the contrary that $h^*(Sz) < \frac{1}{2}S(z,z)$ for some $z \in \mathbb{R}^d$ and take first $z = 0$, so that

$$-h^*(0) = \inf_{y \in \mathbb{R}^d} h(y) > 0.$$ 

Let $u(x) := h(x)1_{\{x\neq 0\}}$ and $\mu \in \mathcal{P}(\mathbb{R}^d)$. We decompose $\mu$ as

$$\mu = t\delta_0 + (1-t)\nu,$$

where $t \in [0,1]$, $\delta_0$ is the Dirac measure at 0, and $\nu \in \mathcal{P}(\mathbb{R}^d)$ is such that $\nu(\{0\}) = 0$. If $t = 1$, then $\mu = \delta_0$ and

$$\mu(u) = \delta_0(u) = u(0) = 0 = \frac{1}{2}S(\delta_0(x),\delta_0(x)) = \frac{1}{2}S(\mu(x),\mu(x)).$$

If $0 \leq t < 1$, then by the convexity of $h$ and the fact that $h \geq 0$,

$$\mu(u) = (1-t)\nu(h) \geq (1-t)h(\nu(x)) \geq \frac{1-t}{2} \max(0,S(\nu(x),\nu(x)))$$

$$= \frac{1}{2(1-t)} \max(0,S(\mu(x),\mu(x))) \geq \frac{1}{2}S(\mu(x),\mu(x)).$$

Implication (a) $\implies$ (b) shows that $\text{cl\ conv} \ u \in \Psi$. As $\text{cl\ conv} \ u \leq u \leq h$ and $u(0) = 0 < h(0)$, we get a contradiction with the minimality of $h$.

The case of general $z$ is reduced to the one above. It is easy to see that the function

$$f(x) = h(x+z) - S(x,z) - \frac{1}{2}S(z,z), \quad x \in \mathbb{R}^d,$$

is a minimal element of $\Psi$. However,

$$f^*(0) = \sup_{x \in \mathbb{R}^d} (-f(x)) = \sup_{x \in \mathbb{R}^d} \left( S(x,z) + \frac{1}{2}S(z,z) - h(x+z) \right)$$

$$= h^*(Sz) - \frac{1}{2}S(z,z) < 0,$$

and we again arrive to a contradiction. \hfill \Box
We are ready to finish the proof of the implication. By Claim 1 we can assume from the start that \( f \) is a minimal element of \( \Psi \). Claim 2 then yields (24). Theorem A.1 shows that

\[
G := \left\{ x \in \mathbb{R}^d \mid f^*(Sx) = \frac{1}{2}S(x, x) \right\} \in \mathcal{M}(S).
\]

Being a closed convex function, \( f \) is the conjugate of \( f^* \). It follows that

\[
f(x) = \sup_{y \in \mathbb{R}^d} (\langle x, Sy \rangle - f^*(Sy)) = \sup_{y \in \mathbb{R}^d} (S(x, y) - f^*(Sy))
\geq \sup_{y \in G} \left( S(x, y) - \frac{1}{2}S(y, y) \right) = \psi_G(x), \quad x \in \mathbb{R}^d.
\]

By Theorem A.2, \( \psi_G \in \Psi \). The minimality of \( f \) implies that \( f = \psi_G \). \( \square \)

Finally, we describe the structure of the subdifferential of \( \psi_G \) in terms of the projection function on \( G \) in the \( S \)-space. Recall from (7) that

\[
P_G(y) := \arg \min_{x \in G} S(x - y, x - y) = \arg \max_{x \in G} \left( S(x, y) - \frac{1}{2}S(x, x) \right)
= \left\{ x \in G \mid \psi_G(y) = S(x, y) - \frac{1}{2}S(x, x) \right\}, \quad y \in \mathbb{R}^d.
\]

The projection \( P_G(y) \) is a closed (possibly empty) subset of \( G \).

For a convex closed set \( C \subset \mathbb{R}^d \) and a point \( x \in C \), we denote by \( N_C(x) \) the normal cone to \( C \) at \( x \):

\[
N_C(x) := \left\{ s \in \mathbb{R}^d \mid \langle s, y - x \rangle \leq 0 \text{ for all } y \in C \right\}.
\]

We recall that \( N_C(x) = 0 \) if and only if \( x \) belongs to the interior of \( C \). Otherwise, \( N_C(x) \) is an unbounded closed convex cone.

For \( A \subset \mathbb{R}^d \), we write

\[
SA := \{ Sx \mid x \in A \}.
\]

**Theorem A.4.** Let \( S \in S_m^d \) and \( G \in \mathcal{M}(S) \). The multi-functions \( P_G \) and \( \partial \psi_G \) have the same domain \( D \) and are related as

\[
P_G(y) = \{ x \in G \mid Sx \in \partial \psi_G(y) \} = \{ x \in G \mid y \in \partial \psi_G^*(Sx) \}.
\]
With \( N_{\Delta D} \) being the normal cone to the closure of \( D \), we have that
\[
\partial \psi_G(y) = \text{cl conv} \left( S \mathcal{P}(y) \right) + N_{\Delta D}(y), \quad y \in D.
\] (30)

In particular, if \( D \) has a nonempty interior, then
\[
\partial \psi_G(y) = \text{conv} \left( S \mathcal{P}(y) \right), \quad y \in \text{int } D = \text{int } \text{dom } \psi_G.
\]

**Proof.** Let \( x, y \in \mathbb{R}^d \). By the properties (3) of subdifferentials of closed convex functions,
\[
Sx \in \partial \psi_G(y) \iff y \in \partial \psi_G(Sx) \iff \psi_G(y) + \psi_G(Sx) = S(x, y).
\]
Theorem A.2 states that \( x \in G \) if and only if \( \psi^*_G(Sx) = \frac{1}{2} S(x, x) \). Formulas (29) for \( P_G(y) \) readily follow.

We denote \( D := \text{dom } \partial \psi_G \). From (29) we deduce that \( \text{dom } P_G \subset D \) and \( S \mathcal{P}(y) \subset \partial \psi_G(y), \ y \in D \). Since
\[
\partial \psi_G(y) = \partial \psi_G(y) + N_{\Delta D}(y), \quad y \in D,
\]
we obtain the inclusion:
\[
\text{cl conv} \left( S \mathcal{P}(y) \right) + N_{\Delta D}(y) \subset \partial \psi_G(y), \quad y \in \text{dom } P_G.
\] (31)

To prove the opposite inclusion, we assume for a moment that
\[
\text{int } D \neq \emptyset.
\]
We recall that \( \text{int } D = \text{int } \text{dom } \psi_G \). We also recall that for \( y \in \text{int } D \), the classical gradient \( \nabla \psi_G(y) \) exists if and only if \( \partial \psi_G(y) \) is a singleton. In this case, \( \partial \psi_G(y) = \{ \nabla \psi_G(y) \} \). We denote
\[
\text{dom } \nabla \psi_G := \{ y \in \text{int } D \mid \nabla \psi_G(y) \text{ exists} \}.
\]

We claim that
\[
S^{-1} \nabla \psi_G(y) \in G, \quad y \in \text{dom } \nabla \psi_G.
\] (32)

If the claim fails for some \( y \in \text{dom } \nabla \psi_G \), then there is \( \epsilon > 0 \) such that
\[
G \subset \left\{ x \in \mathbb{R}^d \mid |x - x_0| \geq \epsilon \right\}.
\]
where \( x_0 := S^{-1} \nabla \psi_G(y) \). As
\[
\psi_G(y) = \sup_{x \in \mathbb{R}^d} (\langle x, y \rangle - \psi_G^*(x)) = \sup_{x \in \mathbb{R}^d} (S(x, y) - \psi_G^*(Sx))
\]
\[
= \langle \nabla \psi_G(y), y \rangle - \psi_G^*(\nabla \psi_G(y)) = S(x_0, y) - \psi_G^*(Sx_0),
\]
the function \( f(x) := \psi_G^*(Sx) - S(x, y) \) attains strict minimum at \( x = x_0 \). The convexity of \( f \) yields that
\[
f(x_0) < \inf_{|x - x_0| \geq \varepsilon} f(x),
\]
and we get the contradiction:
\[
\psi_G(y) > \sup_{|x - x_0| \geq \varepsilon} (S(x, y) - \psi_G^*(Sx)) \geq \sup_{x \in G} \left( S(x, y) - \frac{1}{2} S(x, x) \right) = \psi_G(y).
\]

Now, for \( y \in D \) we denote by \( L(y) \) the set of cluster points of \( \nabla \psi_G \):
\[
L(y) := \{ z = \lim \nabla \psi_G(y_n) \mid \text{dom} \nabla \psi_G \ni y_n \to y \}.
\]
From (29), (32), and the continuity of subdifferentials we obtain that
\[
L(y) \subset SP_G(y), \quad y \in D.
\]

According to [19, Theorem 25.6, p. 246],
\[
L(y) \neq \emptyset \quad \text{and} \quad \partial \psi_G(y) = \text{cl conv} L(y) + N_{clD}(y), \quad y \in D.
\]

It follows that
\[
\partial \psi_G(y) \subset \text{cl conv} (SP_G(y)) + N_{clD}(y), \quad y \in D.
\]

Accounting for (31), we obtain (30). In particular, \( D = \text{dom } P_G \).

To verify the final relation of the theorem, we fix \( y \in \text{int } D \). Then the subdifferential \( \partial \psi_G(y) \) is bounded together with its subset \( SP_G(y) \). As \( SP_G(y) \) is closed, we have that
\[
\text{cl conv} (SP_G(y)) = \text{conv} (SP_G(y)).
\]
Recalling that \( N_{clD}(y) = 0 \) for \( y \in \text{int } D \), we obtain the result.
We have proved (30) under the assumption that $D$ has a nonempty interior. The general case is reduced to this setting by the following arguments.

For $x_0 \in \mathbb{R}^d$, we observe that $\text{dom} \psi_G = x_0 + \text{dom} \psi_{G-x_0}$ and $P_G(y) = x_0 + P_{G-x_0}(y-x_0)$, $\partial \psi_G(y) = Sx_0 + \partial \psi_{G-x_0}(y-x_0)$, $y \in \mathbb{R}^d$.

Therefore, we can assume that $0 \in G \subset \text{dom} \psi_G \subset \text{aff} \text{ dom} \psi_G$. Under this assumption, $F := \text{aff} \text{ dom} \psi_G$ is a linear space. We write $F = E + E'$, where

$$E' := \{ x' \in F \mid S(x', y) = 0, \ y \in F \},$$

$$E := \{ x \in F \mid \langle x, x' \rangle = 0, \ x' \in E' \},$$

and denote by $S_E$ the restriction of the bilinear form $S$ on $E$:

$$S_E(x, y) := S(x, y), \ x, y \in E.$$

The Euclidean projection $G_E$ of $G$ on $E$ is a maximal $S_E$-monotone set and the restriction of the Fitzpatrick function $\psi_G$ to $E$ is the Fitzpatrick function $\psi_{G_E}$ in the $S_E$-space. By construction, $\text{int} \text{ dom} \psi_{G_E} \neq \emptyset$. Therefore, the relation (30) holds for $\psi_{G_E}$ in the $S_E$-space. Being expressed in the original coordinates, this relation takes exactly the form (30).

\[ \square \]

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