# ON OPTIMAL MULTIVARIATE COUPLINGS 

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#### Abstract

As consequence of a characterization of optimal multivariate coupling (transportation) problems we obtain the existence of optimal Monge solutions as well as an explicit construction method for optimal transportation plans in the case that one mass distribution is discrete. We also give a new characterization of an extension of the transportation problem with more than two mass distributions involved.


## 1. c-optimal couplings on $\mathbb{R}^{k}$

The multivariate coupling (transportation) problem on $\mathbb{R}^{k}$ for a transportation 'cost function' $c: \mathbb{R}^{k} \times \mathbb{R}^{k} \rightarrow \mathbb{R}^{1}$ and given mass distributions $P, Q \in M^{1}\left(\mathbb{R}^{k}, \mathbb{B}^{k}\right)$ is defined as the problem

$$
\begin{equation*}
S_{c}(P, Q)=\sup \left\{\int c(x, y) d \mu(x, y) ; \mu \in M(P, Q)\right\} \tag{1.1}
\end{equation*}
$$

where $M(P, Q)$ is the class of all probabilities on $\mathbb{R}^{k} \times \mathbb{R}^{k}$ with marginals $P$ and $Q$. A pair of random variables $X \stackrel{d}{=} P, Y \stackrel{d}{=} Q$ is called c-optimal if

$$
\begin{equation*}
E c(X, Y)=\sup \{E c(U, V) ; U \stackrel{d}{=} P, V \stackrel{d}{=} Q\}=S_{c}(P, Q) \tag{1.2}
\end{equation*}
$$

The calculation of the optimal value $S_{c}(P, Q)$ and the construction of $c$ optimal solutions $(X, Y)$ is a basic problem in probability theory with many interesting applications (cf. Rachev (1991), Cuesta-Albertos, Matran, Rachev and Rüschendorf (1996)). (Note that the corresponding infimum problem can be reduced to the sup problem by switching from $c$ to $-c$.)

The following characterization of optimal solutions given in Rüschendorf (1991) is basic. For its formulation we need some preliminary notions. Call a function $f$ on $\mathbb{R}^{k}$ c-convex if for some index set $I$ and $x_{i} \in \mathbb{R}^{k}, a_{i} \in$ $\mathbb{R}^{1}, i \in I$

$$
\begin{equation*}
f(x)=\sup _{i \in I}\left(c\left(x, y_{i}\right)+a_{i}\right) . \tag{1.3}
\end{equation*}
$$

The $c$-conjugate of a function $f$ is defined by

$$
\begin{equation*}
f^{*}(y)=\sup _{x}(c(x, y)-f(x)), \tag{1.4}
\end{equation*}
$$

the sup being over the domain of $f$. Define the doubly $c$-conjugate

$$
\begin{equation*}
f^{* *}(x)=\sup \left(c(x, y)-f^{*}(y)\right) \tag{1.5}
\end{equation*}
$$

Then $f^{*}$ and $f^{* *}$ are $c$-convex, $f^{* *}$ is the largest $c$-convex function majorized by $f$ and $f=f^{* *}$ if and only if $f$ is $c$-convex. Also $f^{*}, f^{* *}$ are admissible in the sense that

$$
\begin{equation*}
f^{*}(y)+f^{* *}(x) \geq c(x, y) \quad \text { for all } x, y . \tag{1.6}
\end{equation*}
$$

The (doubly) $c$-conjugate functions are basic for the theory of inequalities as in (1.6). The $c$-subgradient of a function $f$ is defined by

$$
\begin{equation*}
\partial_{c} f(x)=\{y ; f(z)-f(x) \geq c(z, y)-c(x, y) \quad \forall z \in \operatorname{dom} f\} \tag{1.7}
\end{equation*}
$$

Let $\mathcal{L}_{m}(P, Q)$ be the set of all lower majorized measurable functions $c=$ $c(x, y)$ i.e. $c(x, y) \geq f_{1}(x)+f_{2}(y)$ for some $f_{1} \in \mathcal{L}^{1}(P)$ and $f_{2} \in L^{1}(Q)$. The following characterization is then to be found in Rüschendorf (1991, 1995).
Theorem 1.1 Let $c \in \mathcal{L}_{m}(P, Q)$ and assume that
$I(c)=\inf \left\{\int h_{1} d P+\int h_{2} d Q ; c \leq h_{1} \oplus h_{2}, h_{1} \in L^{1}(P), h_{2} \in L^{1}(Q)\right\}<\infty$.
a) $X \stackrel{d}{=} P, Y \stackrel{d}{=} Q$ is a c-optimal pair if and only if

$$
\begin{equation*}
Y \in \partial_{c} f(X) \quad \text { a.s. for some } c \text {-convex function } f ; \tag{1.8}
\end{equation*}
$$

b) If $c$ is upper semicontinuous, then there exists an optimal pair $(X, Y)$.

The characterization in (1.8) is equivalent to the condition, that the support $\Gamma$ of $(X, Y)$ is $c$-cyclically monotone, i.e. for all $\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right) \in \Gamma$ and $x_{n+1}:=x_{1}$,

$$
\begin{equation*}
\sum_{i=1}^{n}\left(c\left(x_{i+1}, y_{i}\right)-c\left(x_{i}, y_{i}\right)\right) \leq 0 \tag{1.9}
\end{equation*}
$$

(cf. Knott and Smith (1993) and Ruischendorf (1996)) Some applications of (1.8) and (1.9) can be found in Cuesta-Albertos and Tuero-Diaz (1993),

Rachev (1991), Rüschendorf (1995). If $c(\cdot, y)$ is locally Lipschitz and $P$ has a Lebesgue-density, then for a $c$-optimal pair $(X, Y)$ holds

$$
\begin{equation*}
\nabla f(X)=\nabla_{x} c(X, Y) \quad \text { a.s. } \tag{1.10}
\end{equation*}
$$

(cf. Rüschendorf (1991), formula (73))
We next discuss two consequences of the characterization of coptimal pairs $(X, Y)$.

### 1.1. MONGE FUNCTIONS

The Monge problem is to find an optimal pair of the form $(X, \Phi(X)), X \stackrel{d}{=}$ $P, \Phi(X) \stackrel{d}{=} Q . \Phi$ is then called an optimal Monge function. Since a Monge function $\Phi$ is determined by a nonlinear variational problem even its existence has been an open problem for a long time. Some sufficient conditions for the existence of (optimal) Monge functions have been given in the literature starting with Sudakov(1979) (cf. Cuesta-Albertos and Tuero-Diaz (1993), Gangbo and McCann (1996)). Gangbo and McCann (1996) have shown that an optimal Monge function exists for strictly convex cost functions of the form $c(x, y)=h(x-y)$ if $P$ has a Lebesgue density. We remark that in this case formula (1.10) implies

$$
\begin{equation*}
Y=X-(\nabla h)^{-1}(\nabla f(X)) \quad \text { a.s. } \tag{1.11}
\end{equation*}
$$

the right hand side defines a Monge function $\Phi(X)$. More generally this holds if (1.10) can be resolved uniquely in $Y$.

So the characterization formula (1.8) implies the existence of Monge solutions if $P$ is Lebesgue-continuous and also gives an interesting relation between the gradient of $c$-convex functions $f$ and their $c$-subgradients, the $c$ optimal functions $\Phi$ (cf. also Gangbo and McCann (1996) for an alternative derivation).

### 1.2. EXPLICIT SOLUTIONS FOR DISCRETE $Q$

Let $Q=\sum_{j=1}^{n} \alpha_{j} \varepsilon_{x_{j}}$ be a discrete distribution on $x_{1}, \ldots, x_{n} \in \mathbb{R}^{k}$ then by (1.3) we may restrict our discussion to $c$-convex functions of the form

$$
\begin{equation*}
f(x)=\sup _{1 \leq j \leq n}\left(c\left(x, x_{j}\right)+a_{j}\right) \tag{1.12}
\end{equation*}
$$

Consider the sets $A_{j}=\left\{x ; f(x)=c\left(x, x_{j}\right)+a_{j}\right\}$, then

$$
\begin{equation*}
x_{j} \in \partial_{c} f(x) \text { for } x \in A_{j} . \tag{1.13}
\end{equation*}
$$

The subgradient is not unique only on the boundaries of $A_{j}$. The problem of finding coptimal couplings therefore, is equivalent to finding suitable shifts $a_{j}$ such that

$$
\begin{equation*}
P\left(A_{j}\right)=\alpha_{j}, 1 \leq j \leq n . \tag{1.14}
\end{equation*}
$$

The optimal coupling then is given by $\phi=\sum_{j=1}^{n} x_{j} 1_{A_{j}}$.
If the boundaries of $A_{j}$ have measure zero with respect to $P$ then as a consequence one obtains the existence and uniqueness of an optimal Monge function for this problem. This application of the characterization in (1.8) also has been observed independently in Gangbo and McCann (1996).

In the case that $c(x, y)=-\|x-y\|^{2}$ the boundaries are linear and can be calculated explicitely for $n$ not too large. The following example with $P$ the uniform distribution on the unit square and

$$
Q=\sum_{j=1}^{8} \alpha_{j} \varepsilon_{x_{j}}
$$

has been solved approximatively in Abdellaoui (1994). The following solution is exact. For $\left(\alpha_{1}, \cdots, \alpha_{8}\right)=(0.105,0.2,0.125,0.125,0.125,0.12,0.1,0.1)$ and $\left(x_{1}, \cdots, x_{8}\right)=((0,1),(0.5,0.5),(1,1),(1,0),(0,0),(1,4),(2,3),(1,2))$ one obtains
$\left(a_{1}, \cdots, a_{8}\right)=(0.18,-0.01,0.43,0.05,0,10.86,7.22,2.19)$.
The corresponding optimal partition is given in the following Figure 1:


Figure 1

The corresponding $c$-convex function $f(x)=\sup _{1 \leq j \leq n}\left(c\left(x, x_{j}\right)+a_{j}\right)$ is given in the following Figure 2:


Figure 2
For the cost function $c(x, y)=-\|x-y\|^{4}$ it is more difficult to calculate the volume of the sets $A_{j}$. The following example is for $P$ the uniform distribution on $[0,1]^{2}$ and $Q=\sum_{l=1}^{4} \alpha_{i} \varepsilon_{x_{i}}$ where $\left(\alpha_{1}, \cdots, \alpha_{4}\right)=$ $(0.34,0.05,0.22,0.39),\left(x_{1}, \cdots, x_{4}\right)=((1,1),(0,0),(1,0),(0,1))$. One obtains $\left(a_{1}, \cdots, a_{4}\right)=(0,-0.5,-0.25,0)$


Figure 3

The $c$-convex function corresponding to the optimal solution is given in the following Figure 4:


Figure 4

## 2. A generalized transportation problem

The general duality theorem also holds for cost functions of $n$-variables $c\left(x_{1}, \ldots, x_{n}\right), x_{i} \in \mathbb{R}^{k}$ (cf. Rachev (1991), Rüschendorf (1981)) which are lower majorized (as in Theorem 1)

$$
\begin{align*}
& \sup \left\{\int c\left(x_{1}, \ldots, x_{n}\right) d \mu ; \mu \in M\left(P_{1}, \ldots, P_{n}\right)\right\} \\
& \quad=\inf \left\{\sum_{i=1}^{n} \int f_{i} d P_{i} ; f_{i} \in \mathcal{L}^{1}\left(P_{i}\right) ; c\left(x_{1}, \ldots, x_{n}\right) \leq \sum_{i=1}^{n} f_{i}\left(x_{i}\right)\right\} \tag{2.1}
\end{align*}
$$

where $M\left(P_{1}, \ldots, P_{n}\right)$ is the set of all probability measures on $\mathbb{R}^{k} \times \cdots \times \mathbb{R}^{k}$ with marginals $P_{1}, \ldots, P_{n}$. Not many explicit results are known in this generalized case. Recently Olkin and Rachev (1993) and Knott and Smith (1993) have considered the case $n=3$ and

$$
\begin{equation*}
c(x, y, z):=\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle \tag{2.2}
\end{equation*}
$$

in particular for normal marginals $P_{i}=N\left(0, \Sigma_{i}\right)$.
Note that in this case the problem

$$
\begin{equation*}
\sup \left\{E c(X, Y, Z) ; X \stackrel{d}{=} P_{1}, X \stackrel{d}{=} P_{2}, Z \stackrel{d}{=} P_{3}\right\} \tag{2.3}
\end{equation*}
$$

is equivalent to

$$
\inf \left\{E\|X-Y\|^{2}+\|Y-Z\|^{2}+\|Z-X\|^{2} ; X \stackrel{d}{=} P_{1}, Y \stackrel{d}{=} P_{2}, Z=P_{3}\right\}
$$

and also to

$$
\sup \left\{E\|X+Y+Z\|^{2} ; X \stackrel{d}{=} P_{1}, Y \stackrel{d}{=} P_{2}, Z \stackrel{d}{=} P_{3}\right\}
$$

In the duality theorem (2.1), for the solution of (2.3), we can restrict consideration to convex functions $f_{i}$ (redefining $f_{1}\left(x_{1}\right)$ as sup $\left\{c\left(x_{1}, x_{2}, x_{3}\right)-\right.$ $\left.f_{2}\left(x_{2}\right)-f_{3}\left(x_{3}\right) ; x_{2}, x_{3} \in \mathbb{R}^{k}\right\}$ and similarly $\left.f_{2}, f_{3}\right)$ and, therefore, for an optimal solution $X, Y, Z$ holds:

$$
\begin{equation*}
Y+Z \in \partial f_{1}(X), X+Z \in \partial f_{2}(Y), X+Y \in \partial f_{3}(Z) \tag{2.4}
\end{equation*}
$$

i.e. $Y+Z$ is optimally coupled to $X$, etc. Therefore, with $g_{i}(x)=f_{i}(x)+$ $\frac{1}{2}\|x\|^{2}$ the sum $X+Y+Z$ is also optimally coupled with any of $X, Y, Z$

$$
\begin{equation*}
X+Y+Z \in \partial g_{1}(X) \cap \partial g_{2}(Y) \cap \partial g_{3}(Z) \tag{2.5}
\end{equation*}
$$

For the corresponding minimum problem

$$
\begin{equation*}
\inf \left\{E c(X, Y, Z) ; X \stackrel{d}{=} P_{1}, Y \stackrel{d}{=} P_{2}, Z \stackrel{d}{=} P_{3}\right\} \tag{2.6}
\end{equation*}
$$

one obtains similarly that

$$
\begin{equation*}
Y+Z \in \partial f_{1}(X), X+Z \in \partial f_{2}(Y), X+Y \in \partial f_{3}(Z) \tag{2.7}
\end{equation*}
$$

for some concave functions $f_{i}$ and so again $Y+Z$ is 'optimally' coupled to $X$, etc.

## Remark 2.1

a) Condition (2.7) is not sufficient for optimality as can be seen by the following one dimensional example where $P_{1}=P_{2}=P_{3}=\frac{1}{8} \sum_{i=1}^{8} \varepsilon_{\{i\}}$. Consider random variables $X, Y, Z$ given by permutations (with equal probabilities) $X \simeq\left(\begin{array}{lllll}14238765\end{array}\right) \quad Y \simeq\left(\begin{array}{llllll}3 & 5 & 8 & 4 & 1 & 6\end{array}\right) \quad Z \simeq$ $\left(85421763\right.$ ) (i.e. $P(X=1, Y=3, Z=8)=\frac{1}{8}$ ), then (2.7) is fulfilled. Similarly the triple $U \simeq(13248765), V \simeq(45783216)$ and $W \simeq\left(\begin{array}{llllll}8 & 5 & 1 & 2 & 7 & 3\end{array}\right)$ satisfies (2.7) but $E\|X+Y+Z\|^{2}=$ $E\|U+V+W\|^{2}+1 / 2$.
b) Since $E\|X+Y+Z\|^{2}=E(\langle X, t\rangle+\langle Y, t\rangle+\langle Z, t\rangle)$ with $t=X+Y+Z$ the following approach suggested in Knott and Smith (1994) is promising. Try to find $X \stackrel{d}{=} P_{1}, Y \stackrel{d}{=} P_{2}$ and $Z \stackrel{d}{=} P_{3}$ which are optimal coupled to their sum $t$. In the normal case $P_{i}=N\left(0, \Sigma_{i}\right)$ and if $t \stackrel{d}{=} N\left(0, \Sigma_{0}\right) ; \Sigma_{0}$
nonsingular, it is well known that optimal coupling functions between $t$ and $X_{i}$ are given by

$$
T_{i}=\Sigma_{i}^{1 / 2}\left(\Sigma_{i}^{1 / 2} \Sigma_{0} \Sigma_{i}^{1 / 2}\right)^{-1 / 2} \Sigma_{i}^{1 / 2}
$$

Then the condition $\sum_{i=1}^{3} T_{i}=I$ is easily seen to be equivalent to

$$
\begin{equation*}
\sum_{i=1}^{3}\left(\Sigma_{0}^{1 / 2} \Sigma_{i} \Sigma_{0}^{1 / 2}\right)^{1 / 2}=\Sigma_{0} \tag{2.8}
\end{equation*}
$$

Under the assumption that (2.8) has a positive definite solution Knott and Smith (1993) establish optimality of the triple defined via $T_{i}$. (2.5) gives a justification of this approach of Knott and Smith (1994). If $(X, Y, Z)$ is optimal then without loss in generality we may assume that $(X, Y, Z) \stackrel{d}{=} N(0, \Sigma)$ is jointly optimal. Assuming that $\Sigma_{0}^{*}=$ $\operatorname{Cov}(X+Y+Z)$ is nonsingular we conclude by (2.5) and the uniqueness of optimal couplings in the normal case that equation (2.8) has a solution (namely $\Sigma_{0}^{*}$ ). Positive definiteness of $\Sigma_{0}^{*}$ can be shown for special cases (e.g. the case of commutative $\Sigma_{1}, \Sigma_{2}, \Sigma_{2}$ ) but is an open problem in general.
The following result gives a necessary and sufficient characterization of optimal solutions of (2.2) in general.

Theorem 2.2 Let $X \stackrel{d}{=} P_{1}, Y \stackrel{d}{=} P_{2}$ and $Z \stackrel{d}{=} P_{3}$, let $P_{i}$ have finite covariance matrices, then $(X, Y, Z)$ is optimal for problem (2.2) if and only if there exists a convex, lower semicontinuous function $f$ and a $F$-convex function $g$ with $F(y, z):=f^{*}(y+z)+\langle y, z\rangle$ such that

$$
\begin{array}{ll}
\text { (1) } Y+Z \in \partial f(X) & \text { a.s. }, \\
\text { (2) } Z \in \partial_{F} g(Y) & \text { a.s. } \tag{2.9}
\end{array}
$$

Proof: The duality theorem (2.1) is in the case (2.2)

$$
\begin{align*}
& \sup _{\mu \in M\left(P_{1}, P_{2}, P_{3}\right)} \int(\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle) d \mu(x, y, z) \\
& =\inf \left\{\int f d P_{1}+\int g d P_{2}+\int h d P_{3} ; f(x)+g(y)+h(z)\right. \\
& \geq\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle\} \tag{2.10}
\end{align*}
$$

Assume conditions (1) and (2) and define the $F$-conjugate of $g$ by

$$
\begin{equation*}
h(z):=g^{F}(z)=\sup _{y}\{F(y, z)-g(y)\} \tag{2.11}
\end{equation*}
$$

Then the triple $(f, g, h)$ is admissible, i.e.

$$
\begin{align*}
& f(x)+g(y)+h(z) \\
& \quad=f(x)+g(y)+\sup _{\bar{y}}\left\{f^{*}(\bar{y}+z)+\langle\bar{y}, z\rangle-g(\bar{y})\right\} \\
& =f(x)+g(y)+\sup _{\bar{y}}\left\{\sup _{\bar{x}}\{\langle\bar{x}, \bar{y}+z\rangle-f(\bar{x})\}+\langle\bar{y}, z\rangle-g(\bar{y})\right\} \\
& =f(x)+g(y)+\sup _{\bar{y}}\left\{\sup _{\bar{x}}\{\langle\bar{x}, \bar{y}\rangle+\langle\bar{x}, z\rangle+\langle\bar{y}, z\rangle-f(\bar{x})-g(\bar{y})\}\right\} \\
& \geq f(x)+g(y)+\langle x, y\rangle+\langle x, z\rangle+\langle y, z\rangle-f(x) g(y) \\
& \quad=\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle . \tag{2.12}
\end{align*}
$$

Furthermore, from (1) $Y+Z \in \partial f(X)$ a.s. and, therefore, $f(X)+f^{*}(Y+$ $Z)=\langle X, Y+Z\rangle$ a.s. which implies
$f(X)+f^{*}(Y+Z)+\langle Y, Z\rangle=f(X)+F(Y, Z)=\langle X, Y\rangle+\langle X, Z\rangle+\langle Y, Z\rangle$ a.s.
From (2) $Z \in \partial_{F} g(Y)$ a.s. and so $g(Y)+g^{F}(Z)=F(Y, Z)$ a.s. This implies

$$
\begin{equation*}
f(X)+g(Y)+g^{F}(Z)=\langle X, Y\rangle+\langle Y, Z\rangle+\langle X, Z\rangle \quad \text { a.s. } \tag{2.13}
\end{equation*}
$$

The inequality (2.12) and (2.13) imply optimality, since for any random variables $\tilde{X} \stackrel{d}{=} P_{1}, \tilde{Y} \stackrel{d}{=} P_{2}$ and $\widetilde{Z} \stackrel{d}{=} P_{3}$,

$$
\begin{align*}
& E(\langle\tilde{X}, \tilde{Y}\rangle+\langle\tilde{Y}, \tilde{Z}\rangle+\langle\tilde{X}, \widetilde{Z}\rangle) \\
& \quad \leq E(t(\tilde{X})+g(\tilde{Y})+h(\widetilde{Z})) \\
& \quad=E(t(X)+g(Y)+h(Z)) \\
& \quad=E(\langle X, Y\rangle+\langle Y, Z\rangle+\langle X, Z\rangle) . \tag{2.14}
\end{align*}
$$

For the opposite direction there exist optimal solutions $\left(f_{1}, f_{2}, f_{3}\right)$ of the dual problem. So for an optimal measure $\mu \in M\left(P_{1}, P_{2}, P_{3}\right)$

$$
\begin{equation*}
\int(\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle) d \mu=\int f_{1} d P_{1}+\int f_{2} d P_{2}+\int f_{3} d P_{3} \tag{2.15}
\end{equation*}
$$

where $f_{1}(x)+f_{2}(y)+f_{3}(z) \geq c(x, y, z)$, and equality holds on the support of $\mu$.

Define $f(x)=f_{1}^{* *}(x)=\sup _{y}\left\{\langle x, y\rangle-f_{1}^{*}(y)\right\}$ where $f_{1}^{*}(y)=\sup _{x}\{\langle x, y\rangle-$ $\left.f_{1}(x)\right\}$ is the conjugate. Then $f$ is convex and lower semicontinuous and $f(x) \leq f_{1}(x)$. Define

$$
\begin{aligned}
F(y, z) & :=\sup _{x}\{\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle-f(x)\} \\
& =\sup _{x}\{\langle x, y+z\rangle-f(x)\}+\langle y, z\rangle \\
& =f^{*}(y+z)+\langle y, z\rangle .
\end{aligned}
$$

Then it holds

$$
\begin{aligned}
f_{1}(x)+f_{2}(y)+f_{3}(z) & \geq f(x)+f_{2}(y)+f_{3}(z) \\
\geq f(x)+F(y, z) & \geq\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle .
\end{aligned}
$$

As $\left(f_{1}, f_{2}, f_{3}\right)$ is a solution of the dual problem we obtain

$$
\begin{equation*}
0=\int(f(x)+F(y, z)-(\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle)) d \mu \tag{2.16}
\end{equation*}
$$

and, therefore,

$$
\begin{equation*}
f(x)+F(y, z)=\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle \quad \mu \text { a.s. } \tag{2.17}
\end{equation*}
$$

This implies that

$$
f(x)+f^{*}(y+z)=\langle x, y+z\rangle \quad \mu \text { a.s. }
$$

and, therefore,

$$
Y+Z \in \partial f(X) \quad \text { a.s.. }
$$

For condition (2) define the double $F$-conjugate

$$
g(y)=f_{2}^{F F}(y)=\sup _{z}\left\{F(y, z)-f_{2}^{F}(z)\right\}
$$

where

$$
f_{2}^{F}(z):=\sup _{y}\left\{F(y, z)-f_{2}(y)\right\} .
$$

We have that $g$ is $F$-convex; with

$$
\begin{aligned}
& h(z):=g^{F}(z)\left(=f_{2}^{F}(z)\right) \quad \text { holds (as above) } \\
& f(x)+f_{2}(y)+f_{3}(z) \geq f(x)+g(y)+h(z) \\
& \geq\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle .
\end{aligned}
$$

Again from the optimality equation (2.15)

$$
f(x)+g(y)+h(z)=\langle x, y\rangle+\langle y, z\rangle+\langle x, z\rangle \quad \mu \text { a.s. }
$$

This implies that

$$
g(Y)+h(Z)=F(Y, Z) \quad \text { a.s. }
$$

and, as $h=g^{F}$ it follows that

$$
Z \in \partial_{F} g(Y) .
$$

## Remark 2.3

a) If $g$ is $F$-convex, then $g$ is convex as supremum of the convex functions of the type $f^{*}(\cdot+z)+\langle\cdot, z\rangle+a$. Condition (2) can be reformulated using (1.10) by

$$
\nabla g(Y)=\nabla f^{*}(Y+Z)+Z \quad \text { a.s. }
$$

using continuity of the involved distributions.
Define $h(y):=f^{*}(y)+\frac{1}{2}\|y\|^{2}$, then we obtain

$$
\begin{equation*}
(\nabla h)^{-1}(\nabla g(Y)+Y)-Y=Z \tag{2.18}
\end{equation*}
$$

b) An analog result holds true for the inf-problem

$$
\begin{equation*}
\inf _{X, Y, Z} E(\langle X, Y\rangle+\langle Y, Z\rangle+\langle X, Z\rangle) \tag{2.19}
\end{equation*}
$$

The corresponding characterizations are: $(X, Y, Z)$ is optimal for (2.17)

$$
\begin{align*}
\Leftrightarrow & \text { (1) } Y+Z \in-\partial(-f)(X) \\
& \text { (2) } Z \in \partial_{-F}-g(Y) \tag{2.20}
\end{align*}
$$

where $f$ is concave, $f^{*}$ the concave conjugate and $g$ is $F$-concave.
Example 2.4 Consider the univariate example $P_{1}=P_{2}=P_{3}=U([0,1])$ the uniform distribution on $[0,1]$. Then the inf problem (2.17) is solved by $\left(X, \Phi_{1}(X), \Phi_{2}(X)\right)$, where

$$
\begin{align*}
& X \stackrel{d}{=} U([0,1]), \quad \Phi_{1}(x):= \begin{cases}1-2 x, & x \leq \frac{1}{2} \\
2-2 x, & x>\frac{1}{2}\end{cases}  \tag{2.21}\\
& \Phi_{2}(x):= \begin{cases}x+\frac{1}{2}, & x \leq \frac{1}{2} \\
x-\frac{1}{2}, & x>\frac{1}{2}\end{cases}
\end{align*}
$$

For the proof define $f(x):=\frac{3}{2} x-\frac{1}{2} x^{2}=g(x)$. Then $f$ is concave and

$$
-\partial(-f(x))=f^{\prime}(x)=\frac{3}{2}-x=\Phi_{1}(x)+\Phi_{2}(x)
$$

and, therefore,

$$
\begin{equation*}
\Phi_{1}(x)+\Phi_{2}(x) \in-\partial(-f(x)) \tag{2.22}
\end{equation*}
$$

i.e. condition (1).

Further,

$$
\begin{aligned}
f^{*}(x) & =\inf _{y}\{x y-f(y)\} \\
& =\inf _{y}\left\{x y-\frac{3}{2} y+\frac{1}{2} y^{2}\right\}=-\frac{1}{2}\left(\frac{3}{2}-x\right)^{2} .
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
F(y, z) & =f^{*}(y+z)+y z \\
& =-\frac{9}{8}+\frac{3}{2} y+\frac{3}{2} z-\frac{1}{2} y^{2}-\frac{1}{2} z^{2}-y z+y z \\
& =g(y)+g(z)-\frac{9}{8}
\end{aligned}
$$

This implies

$$
\begin{equation*}
F\left(y^{\prime}, z\right)-F(y, z)=g\left(y^{\prime}\right)-g(y) . \tag{2.23}
\end{equation*}
$$

Since $g(y)=F(y, z)-g(z)+\frac{9}{8}, g$ is $F$ concave and $z \in \partial_{F} g(y)$. Therefore, the second condition $\Phi_{2}(x) \in \partial_{-F}-g\left(\Phi_{1}(x)\right)$ is fulfilled and the optimality is established by (2.18).

As consequence of the characterization in Theorem 2.2 one obtains the following more specific coupling property of an optimal pair in problem (2.3) to the sum.

Proposition 2.5 If $(X, Y, Z)$ is an optimal solution for $\sup \{E\langle X, Y\rangle+$ $\langle Y, Z\rangle+\langle X, Z\rangle\}$ then for the following convex functions $f_{1}, f_{2}, f_{3}$ given (in the notation of Theorem 2.2) by $f_{1}(x)=f(x)+\frac{1}{2}\|x\|^{2}, \quad f_{2}(x)=g(x)+$ $\frac{1}{2}\|x\|^{2}$ and $f_{3}(x)=g^{F}(x)+\frac{1}{2}\|x\|^{2}$.

$$
\begin{array}{lll}
\text { (1) } & X+Y+Z \in \partial f_{1}(X) & \text { a.s. } \\
\text { (2) } & X+Y+Z \in \partial f_{2}(Y) & \text { a.s. } \\
\text { (3) } & X+Y+Z \in \partial f_{3}(Z) & \text { a.s. }
\end{array}
$$

i.e. $X, Y, Z$ are optimally coupled to the sum.

Proof: From (2.9) in Theorem $2.2 Y+Z \in \partial f(X)$ and, therefore, for any $x^{\prime}$

$$
\begin{aligned}
\left\langle X+Y+Z, X-x^{\prime}\right\rangle & =\left\langle Y+Z, X-x^{\prime}\right\rangle+\left\langle X, X-x^{\prime}\right\rangle \\
& \geq f(X)-f\left(x^{\prime}\right)+\frac{1}{2}\|X\|^{2}-\frac{1}{2}\left\|x^{\prime}\right\|^{2} .
\end{aligned}
$$

This implies $X+Y+Z \in \partial f_{1}(X)$.
Since $X \in \partial f^{*}(Y+Z)$

$$
\langle X, Y+Z-\xi\rangle \geq f^{*}(Y+Z)-f^{*}(\xi), \forall \xi .
$$

Therefore, from (2.9) relation (2):
$F(Y, Z)-F\left(y^{\prime}, Z\right)=f^{*}(Y+Z)-f^{*}\left(y^{\prime}+Z\right)+\left\langle Y-y^{\prime}, Z\right\rangle \geq g(Y)-g\left(y^{\prime}\right)$.
$g$ is convex by Remark 2.2a) and as $\left\langle X+Z, Y-y^{\prime}\right\rangle=\left\langle X, Y+Z-\left(y^{\prime}+Z\right)\right\rangle+$ $\left\langle Y-y^{\prime}, Z\right\rangle \geq f^{*}(Y+Z)-f^{*}\left(y^{\prime}+Z\right)+\left\langle Y-y^{\prime}, Z\right\rangle$ we obtain $X+Z \in \partial g(Y)$ and, therefore, $X+Y+Z \in \partial f_{2}(Y)$ a.s.

Finally, from (2) in (2.9) $Y \in \partial_{F} g^{F}(Z)$. The $F$ conjugate of $g$ is convex. Then we can argue as a above to obtain $X+Y+Z \in \partial f_{3}(Z)$.

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