(Probably) Concave Graph Matching

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Abstract
In this paper, we address the graph matching problem. Following the recent works of Zaslavskiy et al. (2009); Vestner et al. (2017) we analyze and generalize the idea of concave relaxations. We introduce the concepts of conditionally concave and probably conditionally concave energies on polytopes and show that they encapsulate many instances of the graph matching problem, including matching Euclidean graphs and graphs on surfaces. We further prove that local minima of probably conditionally concave energies on general matching polytopes (e.g., doubly stochastic) are with high probability extreme points of the matching polytope (e.g., permutations).

1 Introduction
Graph matching is a generic and popular modeling tool for problems in computational sciences such as computer vision (Berg et al., 2005; Zhou and De la Torre, 2012; Rodola et al., 2013; Bernard et al., 2017), computer graphics (Funkhouser and Shilane, 2006; Kezurer et al., 2015), medical imaging (Guo et al., 2013), and machine learning (Umeyama, 1988; Huet et al., 1999; Cour et al., 2007). In general, graph matching refers to several different optimization problems of the form:

$$\min_X E(X) \text{ s.t. } X \in \mathcal{F}$$

where $\mathcal{F} \subseteq \mathbb{R}^{n \times n_0}$ is a collection of matchings between vertices of two graphs $G_A$ and $G_B$, and $E(X) = [X]^T M [X] + a^T [X]$ is usually a quadratic function in $X \in \mathbb{R}^{n \times n_0}$ ($[X] \in \mathbb{R}^{n_0 \times 1}$ is its column stack). Often, $M$ quantifies the discrepancy between edge affinities exerted by the matching $X$. Edge affinities are represented by symmetric matrices $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n_0 \times n_0}$. Maybe the most common instantiation of (1) is

$$E_1(X) = \|AX - XB\|^2_F$$

and $\mathcal{F} = \Pi_n$, the matrix group of $n \times n$ permutations. The permutations $X \in \Pi_n$ represent bijections between the set of $(n)$ vertices of $G_A$ and the set of $(n)$ vertices of $G_B$. We denote this problem as GM. From a computational point of view, this problem is equivalent to the quadratic assignment problem, and as such is an NP-hard problem (Burkard et al., 1998). A popular way of obtaining approximate solutions is by relaxing its combinatorial constraints (Loiola et al., 2007).

A standard relaxation of this formulation (e.g. Almohamad and Duffuaa (1993); Afflalo et al. (2015); Fiori and Sapiro (2015)) is achieved by replacing $\Pi_n$ with its convex hull, namely the set of doubly-stochastic matrices $\text{DS} = \text{hull}(\mathcal{F}) = \{ X \in \mathbb{R}^{n \times n} \mid X1 = 1, X^T 1 = 1, X \geq 0 \}$. The main advantage of this formulation is the convexity of the energy $E_1$; the main drawback is that often the minimizer is not a permutation and simply projecting the solution onto $\Pi_n$ doesn’t take the energy into account resulting in a suboptimal solution. The prominent Path Following algorithm (Zaslavskiy et al., 2009) suggests a better solution of continuously changing $E_1$ to a concave energy $E'$ that coincide (up to an additive constant) with $E_1$ over the permutations. The concave energy $E'$ is called concave relaxation and enjoys three key properties: (i) Its solution set is the same as the GM problem. (ii) Its set of local optima are all permutations. This means no projection of the local optima onto the permutations is required. (iii) For every descent direction, a maximal step is always guaranteed to reduce the energy most.
A surprising fact we show is that probably conditionally concave energies are pretty common and
where
\[ \{ \Phi : \mathbb{R}^d \rightarrow \mathbb{R} \} \]
produce positive (negative) definite matrices when restricted to certain linear subspaces; this notion will be
formally introduced and defined in Section 2.

Let \( M \) be both conditionally positive (or negative) definite functions of order 1. For any pair of graphs with affinity matrices \( A, B \in \mathbb{R}^{n \times n} \) so that
\[ A_{ij} = \Phi(x_i - x_j), \quad B_{ij} = \Psi(y_i - y_j) \]
for some arbitrary \( \{ x_i \}_{i \in [n]} \subset \mathbb{R}^d, \{ y_i \}_{i \in [n]} \subset \mathbb{R}^s \), the energy \( E_2(X) \) is conditionally concave, i.e.,
its Hessian \( M|_{\text{lin}(DS)} \prec 0 \).

One useful application of this theorem is in matching graphs with Euclidean affinities, since Euclidean
distances are conditionally negative definite of order 1 (Wendland, 2004). That is, the affinities are
Euclidean distances of points in Euclidean spaces of arbitrary dimensions,
\[ A_{ij} = \| x_i - x_j \|_2, \quad B_{ij} = \| y_i - y_j \|_2, \]
where \( \{ x_i \}_{i \in [n]} \subset \mathbb{R}^d, \{ y_i \}_{i \in [n]} \subset \mathbb{R}^s \). This class contain, besides Euclidean graphs, also affinities
made out of distances that can be isometrically embedded in Euclidean spaces such as diffusion
distances (Coifman and Lafon, 2006), distances induced by deep learning embeddings (e.g. Schroff
et al., 2015) and Mahalanobis distances. Furthermore, as shown in Bogomolny et al. (2007) the
spherical distance, \( A_{ij} = d_{s,t}(x_i, x_j) \), is also conditionally negative definite over the sphere and
therefore can be used in the context of the theorem as well.

Second, we generalize the notion of conditionally concave energies to probably conditionally concave
energies. Intuitively, the energy \( E \) is called probably conditionally concave if it is rare to find a linear
subspace \( D \) of \( \text{lin}(DS) \) so that the restriction of \( E \) to it is convex, that is \( M|_D \succeq 0 \). The primary motivation in considering probably conditionally concave energies is that they enjoy (with high probability) the same properties as the conditionally concave energies, i.e., (i)-(iii). Therefore, locally minimizing probably conditionally concave energies over \( F \) can be done also with the Frank-Wolfe algorithm, with guarantees (in probability) on the feasibility of both the optimization result and the solution set of this energy.

A surprising fact we show is that probably conditionally concave energies are pretty common and
include Hessian matrices \( M \) with almost the same ratio of positive to negative eigenvalues. The

\[ E_2(X) = -\text{tr}(BX^TAX) \]
over the doubly-stochastic matrices, DS, as well. Note that both energies \( E_1, E_2 \) are identical (up to an additive constant) over the permutations and hence both are considered relaxations. However, in contrast to \( E_1, E_2 \) is in general indefinite, resulting in a non-convex relaxation. Vogelstein et al., 2015; Lyzinski et al. 2016; Vestner et al., 2017; Boyarski et al., 2017] have considered the energy

\[ E_2(X) = -\text{tr}(BX^TAX) \]
in a nutshell, positive (negative) definite functions are functions that when applied to differences of vectors
produce positive (negative) definite matrices when restricted to certain linear subspaces; this notion will be
formally introduced and defined in Section 2.
The chance that a local minimum of $\min_{X \in \mathcal{F}} E(X)$ is outside $\Pi_n$ is extremely small, bounded by $\exp(-c_1 n^2)$, for some constant $c_1 > 0$.

Third, when the energy of interest $E(X)$ is not probably conditionally concave over $\text{lin}(\mathcal{F})$ there is no guarantee that the local optimum of $E$ over $\text{hull}(\mathcal{F})$ is in $\mathcal{F}$. We devise a simple variant of the Frank-Wolfe algorithm, replacing the standard line search with a concave search. Concave search means subtracting from the energy $E$ convex parts that are constant on $\mathcal{F}$ (i.e., relaxations) until an energy reducing step is found.

2 Conditionally concave energies

We are interested in the application of the Frank-Wolfe algorithm\cite{Frank1956} for locally optimizing $E_2$ (potentially with a linear term) from\cite{Lyzinski2016} over the doubly-stochastic matrices:

$$\min_{X} E(X)$$

subject to $X \in \text{DS}$

where $E(X) = -[X]^T (B \otimes A) [X] + a^T [X]$. For completeness, we include a simple pseudo-code:

```
input: X_0 \in \text{hull}(\mathcal{F})
while not converged do
    compute step: X_1 = \min_{X \in \text{DS}} -2[X_0]^T (B \otimes A) [X] + a^T [X];
    line-search: t_0 = \arg\min_{t \in [0,1]} E((1-t)X_0 + tX_1);
    apply step: X_0 = (1-t_0)X_0 + t_0X_1;
end
```

Algorithm 1: Frank-Wolfe algorithm.

**Definition 1.** We say that $E(X)$ is conditionally concave if it is concave when restricted to the linear space $\text{lin}(\mathcal{F})$, the linear part of the affine-hull $\text{hull}(\mathcal{F})$. 


If $E(X)$ is conditionally concave we have that properties (i)-(iii) of concave relaxations detailed above hold. In particular Algorithm\cite{Wendland2004} would always accept $t_0 = 1$ as the optimal step, and therefore it will produce a series of feasible matchings $X_0 \in \Pi_n$ and will converge after a finite number of steps to a permutation local minimum $X_* \in \Pi_n$ of (8). Our first result in this paper provides sufficient condition for $W = -B \otimes A$ to be concave. It provides a connection between conditionally positive (or negative) definite functions \cite{Wendland2004}, and negative definiteness of $-B \odot A$:

**Definition 2.** A function $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is called conditionally positive definite of order $m$ if for all pairwise distinct points $\{x_i\}_{i \in [n]} \subset \mathbb{R}^d$ and all $0 \neq \eta \in \mathbb{R}^n$ satisfying $\sum_{i \in [n]} \eta_i \Phi(x_i) = 0$ for all $d$-variate polynomials $p$ of degree less than $m$, we have $\sum_{i,j=1}^n \eta_i \eta_j \Phi(x_i - x_j) > 0$.

Specifically, $\Phi$ is conditionally positive definite of order 1 if for all pairwise distinct points $\{x_i\}_{i \in [n]} \subset \mathbb{R}^d$ and zero-sum vectors $0 \neq \eta \in \mathbb{R}^d$ we have $\sum_{i,j=1}^n \eta_i \eta_j \Phi(x_i - x_j) > 0$. Conditionally negative definiteness is defined analogously. Some well-known functions satisfy the above conditions, for example: $-\|x\|_2$, $-(c^2 + \|x\|_2^2)^\beta$ for $\beta \in (0, 1]$ are conditionally positive definite of order 1, while the functions $\exp(-\tau^2\|x\|_2^2)$ for all $\tau$, and $c_{\beta_0} = (1 - \|x\|_2^2)$ are conditionally positive definite of order 0 (also called just positive definite functions). Note that if $\Phi$ is conditionally positive definite of order $m$, it is also conditionally positive definite of any order $m' > m$. Lastly, as shown in \cite{Bogomolny2007}, spherical distances $-d(x, x')$ are conditionally positive semidefinite for $\gamma \in (0, 1]$, and $\exp(-\tau d(x, x')^\gamma)$ are positive definite for $\gamma \in (0, 1]$ and all $\tau$. We now prove:

**Theorem 1.** Let $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$, $\Psi : \mathbb{R}^s \rightarrow \mathbb{R}$ be both conditionally positive (or negative) definite functions of order 1. For any pair of graphs with affinity matrices $A, B \in \mathbb{R}^{n \times n}$ so that

$$A_{ij} = \Phi(x_i - x_j), \quad B_{ij} = \Psi(y_i - y_j)$$

for some arbitrary $\{x_i\}_{i \in [n]} \subset \mathbb{R}^d$, $\{y_i\}_{i \in [n]} \subset \mathbb{R}^s$, the energy $E_2(X)$ is conditionally concave, i.e., its Hessian $M|_{\text{lin}(DS)} < 0$.

**Lemma 1** (orthonormal basis for $\text{lin}(DS)$). If the columns of $F \in \mathbb{R}^{n \times (n-1)}$ constitute an orthonormal basis for the linear space $1^\perp = \{x \in \mathbb{R}^n \mid x^T 1 = 0\}$ then the columns of $F \otimes F$ are an orthonormal basis for $\text{lin}(DS)$.

**Proof.** First, \((F \otimes F)^T(F \otimes F) = (F^T \otimes F^T)(F \otimes F) = (F^T F) \otimes (F^T F) = I_{n-1} \otimes I_{n-1} = I_{(n-1)^2}\). Therefore $F \otimes F$ is full rank with $(n-1)^2$ orthonormal columns. Any column of $F \otimes F$ is of the form $F_i \otimes F_j$, where $F_i, F_j$ are the $i$th and $j$th columns of $F$, respectively. Now, reshaping $F_i \otimes F_j$ back into an $n \times n$ matrix using the inverse of the bracket operation we get $X = [F_i \otimes F_j]^T = F_i^T F_j^T$ which are clearly in $\text{lin}(DS)$. Lastly, since the dimension of $\text{lin}(DS)$ is $(n-1)^2$ the lemma is proved.

**Proof.** (of Theorem\cite{Wendland2004}) Let $A, B \in \mathbb{R}^{n \times n}$ be as in the theorem statement. Checking that $E(X)$ is conditionally concave amounts to restricting the quadratic form $-X^T (B \odot A) X$ to $\text{lin}(DS)$: $-(F \otimes F)^T(B \odot A)(F \otimes F) = -(F^T BF) \otimes (F^T AF) < 0$, where we used Lemma\cite{Wendland2004} and the fact that $\Phi, \Psi$ are conditionally positive definite of order 1.

**Corollary 1.** Let $A, B$ be Euclidean distance matrices then the solution set of Problem\cite{Wendland2004} and GM coincide.

### 3 Probably conditionally concave energies

Although Theorem\cite{Wendland2004} covers a rather wide spectrum of instantiations of Problem\cite{Wendland2004} it definitely does not cover all interesting scenarios. In this section we would like to consider a more general energy $E(X) = [X]^T M[X] + a^T [X], \; X \in \mathbb{R}^{n \times n}, \; M \in \mathbb{R}^{n^2 \times n^2}$ and the optimization problem:

$$\min_X \quad E(X)$$

subject to $X \in \text{hull}(\mathcal{F})$

We assume that $\mathcal{F} = \text{ext}(\text{hull}(\mathcal{F}))$, namely, the matchings are extreme points of their convex hull (as happens e.g., for permutations $F = \Pi_n$). When the restricted Hessians $M|_{\text{lin}(\mathcal{F})}$ are $\epsilon$-negative definite (to be defined soon) we will call $E(X)$ probably conditionally concave.
We first make some preparations. Recall the definition of the Grassmannian $X$ where the last equality follows from the independence of what else this definition encapsulates:

For a subset $X$ is known to be (1\footnote{with no line search (t0 = 1) and achieve local minima in $F$ (no post-processing is required). In addition, we prove that certain classes of conditionally concave relaxations have no local minima that are outside $F$, with high probability. In the experiment section we will also demonstrate that in practice this algorithm works well for different choices of conditionally concave energies. Popular energies that fall into this category are, for example, with $A, B$ geodesic distance matrices or certain functions thereof.}

We first make some preparations. Recall the definition of the Grassmannian $G_r(d, m)$: It is the set of $d$-dimensional linear subspaces in $\mathbb{R}^m$; it is a compact differential manifold defined by the quotient $O(m)/O(d) × O(m - d)$, where $O(s)$ is the orthogonal group in $\mathbb{R}^s$. The orthogonal group $O(m)$ acts transitively on $G_r(d, m)$ by taking an orthogonal basis of any $d$-dimensional linear subspace to an orthogonal basis of a possibly different $d$-dimensional subspace. On $O(m)$ there exists Haar probability measure, that is a probability measure invariant to actions of $O(m)$. The Haar probability measure on $O(m)$ induces an $O(m)$-invariant (which we will also call Haar) probability measure on $G_r(d, m)$.

We now introduce the notion of $\epsilon$-negative definite matrices:

**Definition 3.** A symmetric matrix $M \in \mathbb{R}^{m \times m}$ is called $\epsilon$-negative definite if the probability of finding a $d$-dimensional linear subspace $D \in G(d, m)$ so that $A$ is convex over $D$ is smaller than $\epsilon^d$.

That is, $P_r(M|\mathcal{D}) \leq \epsilon^d$ where the probability is taken with respect to a Haar $O(m)$-invariant measure on the Grassmannian $G_r(d, m)$.

One way to interpret $M|\mathcal{D}$, the restriction of the matrix $M$ to the linear subspace $D$, is to consider a matrix $F \in \mathbb{R}^{m \times d}$ where the columns of $F$ form a basis to $D$ and consider $M|D = F^T MF$. Clearly, negative definite matrices are $\epsilon$-negative definite for all $\epsilon > 0$.

The following theorem helps to see what else this definition encapsulates:

**Theorem 2.** Let $M \in \mathbb{R}^{m \times m}$ be a symmetric matrix with eigenvalues $\lambda_1, \ldots, \lambda_m$. Then, for all $t \in (0, \frac{1}{\lambda_{\text{max}}})$:

$$P_r(M|D \geq 0) \leq \prod_{i=1}^m (1 - 2t\lambda_i)^{-\frac{d}{2}},$$

where $M|D$ is the restriction of $M$ to the $d$-dimensional linear subspace defined by $D \in G_r(d, m)$ and the probability is taken with respect to the Haar probability measure on $G_r(d, m)$.

**Proof.** Let $F$ be an $m \times d$ matrix of i.i.d. standard normal random variables $\mathcal{N}(0, 1)$. Let $F_j, j \in [d]$, denote the $j$th column of $F$. The multivariate distribution of $F$ is $O(m)$-invariant in the sense that for a subset $A \subset \mathbb{R}^{m \times d}$, $P_r(RA) = P_r(A)$ for all $R \in O(m)$. Therefore, $P_r(M|D \geq 0) = P_r(F^T MF \geq 0)$. Next, $P_r(F^T MF \geq 0) \leq P_r(\bigcap_{j=1}^d \{ F_j^T MF_j \geq 0 \}) = \prod_{j=1}^d P_r(F_j^T MF_j \geq 0)$, where the inequality is due to the fact that a positive semidefinite matrix necessarily has nonnegative diagonal, and the equality is due to the independence of the random variables $F_j^T MF_j$, $j \in [d]$. We now calculate the probability $P_r(F_1^T MF_1)$ which is the same for all columns $j \in [d]$. For brevity let $X = (X_1, X_2, \ldots, X_m)^T = F_1$. Let $M = U\Lambda U^T$, where $U \in O(m)$ and $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$ be the spectral decomposition of $M$. Since $UX$ has the same distribution as $X$ we have that $P_r(X^T MX \geq 0) = P_r(X^T \Lambda X \geq 0) = P_r(\sum_{j=1}^m \lambda_j X_i^2 \geq 0)$. Since $X_i^2 \sim \chi^2(1)$ we have transformed the problem into a non-negativity test of a linear combination of chi-squared random variables. Using the Chernoff bound we have for all $t > 0$:

$$P_r \left( \sum_{i=1}^m \lambda_i X_i^2 \geq 0 \right) \leq \mathbb{E} \left( e^{t \sum_{i=1}^m \lambda_i X_i^2} \right) = \prod_{i=1}^m \mathbb{E} \left[ e^{t \lambda_i X_i^2} \right],$$

where the last equality follows from the independence of $X_1, \ldots, X_m$. To finish the proof we note that $\mathbb{E} \left[ e^{t \lambda_i X_i^2} \right]$ is the moment generating function of the random variable $X_i^2$ sampled at $t\lambda_i$ which is known to be $(1 - 2t\lambda_i)^{-1/2}$ for $t\lambda_i < \frac{1}{2}$ which means that we can take $t < \frac{1}{2\lambda_i}$ when $\lambda_i \neq 0$ and disregard all $\lambda_i = 0$.

Theorem 2 shows that there is a concentration of measure phenomenon when the dimension $m$ of the matrix $M$ increases. For example consider:

$$\Lambda_{m,p} = \left( \frac{(1-p)m}{\Lambda_1, \Lambda_2, \ldots, \mu_1, \mu_2, \ldots} \right),$$

(12)
Another consequence that comes out of this theorem (in fact, its proof) is that the probability of
where
\[ \lambda_i \leq -b, b > 0 \] are the negative eigenvalues; \( 0 \leq \mu_i \leq a, a > 0 \) are the positive eigenvalues
and the ratio of positive to negative eigenvalues is a constant \( p \in (0, 1/2) \). We can bound the r.h.s. of
\( (11) \) with \( (1 + 2bt)^{-\frac{a-bp}{b}} (1 - 2at)^{-\frac{ap}{2}} \). Elementary calculus shows that the minimum of this
function over \( t \in (0, 1/2a) \) gives:
\[
P_r(v^tMv \geq 0) \leq \left( \frac{a^1-pbp}{a+b} \frac{1}{2}(1-p)p^{p-1}p^{-p} \right)^{\frac{m}{2}}, \tag{13}
\]
where \( v \) is uniformly distributed on the unit sphere in \( \mathbb{R}^m \). The function \( \frac{1}{2}(1-p)p^{p-1}p^{-p} \) is shown in the inset and for \( p < 1/2 \) it is strictly smaller
than 1. The term \( \frac{a^1-pbp}{a+b} \) is the ratio of the weighted geometric mean and the arithmetic mean.
Using the weighted arithmetic-geometric inequality it can be shown that these terms is at-most 1 if \( a \leq b \). To summarize, if \( a \leq b \) and \( p < 1/2 \) the probability to find a convex (positive) direction in \( M \) is exponentially decreasing in \( m \),
the dimension of the matrix. One simple example is taking \( a = b = 1, p = 0.49 \) which shows that
considering the matrices
\[
0.51m \quad 0.49m
\]
\[ U(-1,-1,\ldots,-1,1,1,\ldots,1)U^T \]
it will be extremely hard to get in random a convex direction in dimension \( m \approx 300^2 \), i.e., the
probability will be \( \approx 4 \cdot 10^{-5} \) (this is a low dimension for a matching problem where \( m = (n-1)^2 \)).
Another consequence that comes out of this theorem (in fact, its proof) is that the probability of
finding a linear subspace \( D \in G_r(d,m) \) for which the matrix \( M \) is positive semidefinite is bounded
by the probability of finding a one-dimensional subspace \( D_1 \in G_r(1,m) \) to the power of \( d \). Therefore
the \( d \) exponent in Definition\[3\] makes sense. Namely, to show a symmetric matrix \( M \) is \( \epsilon \)-negative
definite it is enough to check one-dimensional linear subspaces. An important implication of this fact
and one of the motivations for Definition\[3\] is that finding local minima at high dimensional faces
of the polytope \( \text{hull}(F) \) is much less likely than at low dimensional faces.

Next, we would like to prove Theorem\[3\] that shows that for natural probability space of Hessians
\( \{\Omega\} \) the local minima of \( (10) \) are with high probability in \( F \), e.g., permutations in case that
\( F = \Pi_n \). We therefore need to devise a natural probability space of Hessians. We opt to consider Hessians of
the form discussed above, namely
\[
\Omega_m = \{ U\Lambda_{m,p}U^T \mid U \in O(m) \}, \tag{14}
\]
where \( \Lambda_{m,p} \) is defined in \( (12) \). The probability measure over \( \Omega_m \) is defined using the
Haar probability measure on \( O(m) \), that is for a subset \( A \subset \Omega_m \) we define
\[ Pr\{ A \} = Pr\{ U \in O(m) \mid U\Lambda_{m,p}U^T \in A \} \]
where the probability measure on the r.h.s. is the probability Haar measure on \( O(m) \). Note that \( (14) \) is plausible since the input graphs \( G_A, G_B \) are usually provided with an arbitrary ordering of the vertices. Writing the quadratic energy
\( E \) resulted from a different ordering \( P, Q \in \Pi_n \) of the vertices of \( G_A, G_B \) (resp.) yields the Hessian
\( H' = (Q \otimes P)(B \otimes A)(Q \otimes P)^T \), where \( Q \otimes P \in \Pi_m \subset O(m) \). This motivates defining a Hessian
probability space that is invariant to \( O(m) \). We prove:

**Theorem 3.** *If the number of extreme points of the polytope \( \text{hull}(F) \) is bounded by \( \exp(m^{1-\epsilon}) \), for
some fixed arbitrary \( \epsilon > 0 \), and the Hessian of \( E \) is drawn from the probability space \( (\Omega_m, Pr) \), the
certainty that a local minimum of \( \min_{X \in \text{hull}(F)} E(X) \) is outside \( F \) is extremely small, bounded by
\( \exp(-c_1m) \), for some constant \( c_1 > 0 \).*

**Proof.** Denote all the edges (i.e., one-dimensional faces) of the polytope \( P = \text{hull}(F) \) by indices \( \alpha \).
Even if every two extreme points of \( P \) are connected by an edge there could be at most \( \exp(2m^{1-\epsilon}) \)
edges. A local minimum \( X_\alpha \in P \) to \( (10) \) that is not in \( F \) necessarily lies in the (relative) interior of
some face \( f \) of \( P \) of dimension at-least one. The restriction of the Hessian \( M \) of \( E(X) \) to \( \text{lin}(f) \) is
therefore necessarily positive semidefinite. This implies there is a direction \( v_\alpha \in \mathbb{R}^m \), parallel to an
edge \( \alpha \) of \( P \) so that \( v_\alpha^TMv_\alpha \geq 0 \).

Let us denote by \( X_\alpha \) the indicator random variable that equals one if \( v_\alpha^TMv_\alpha \geq 0 \) and zero otherwise.
If \( X_\alpha = 1 \) we say that the edge \( \alpha \) is a critical edge for \( M \). Let us denote \( X = \sum_\alpha X_\alpha \) the random
variable counting critical edges. The expected number of critical edges is \( E(X) = \sum_\alpha Pr(v_\alpha^TMv_\alpha \geq 0) \). We use Theorem\[2\] in particular \( (15) \), to bound the summands.
Since \( P_r(v_a^T M v_a \geq 0) = P_r(v_a^T U A_m, p U^T v_a \geq 0) \) and \( U^T v_a \) is distributed uniformly on the unit sphere in \( \mathbb{R}^m \), we can use (13) to infer that \( P_r(v_a^T M v_a \geq 0) \leq \eta^{m/2} \) for some \( \eta \in [0,1] \) and therefore \( \mathbb{E}(X) \leq \exp(m \log \eta/2) \sum_{\eta} 1 \) (note that \( \log \eta < 0 \)). Incorporating the bound on edge number in \( P \) discussed above we get \( \mathbb{E}(X) \leq \exp(\log \frac{1}{2} m + 2m_{1-r}) \leq \exp(-c_1 m) \) for some constant \( c_1 > 0 \). Lastly, as explained above, the event of a local minimum not in \( F \) is contained in \( X \geq 1 \) and by Markov’s inequality we finally get \( P_r(X \geq 1) \leq \mathbb{E}(X) \leq \exp(-c_1 m) \). 

Let us use this theorem to show that the local optimal solutions to Problem (10) with permutations as matchings, \( F = \Pi_n \), are with high probability permutations:

**Theorem 4.** Let \( E \) be a quadratic energy with Hessian drawn from the probability space \( (\Omega_m, P_r) \). The chance that a local minimum of \( \min_{X \in DS} E(X) \) is outside \( \Pi_n \) is extremely small, bounded by \( \exp(-c_1 n^2) \), for some constant \( c_1 > 0 \).

**Proof.** In this case the polytope \( DS = \text{hull}(\Pi_n) \) is in the \((n-1)^2\) dimensional linear subspace \( \text{lin}(DS) \) of \( \mathbb{R}^{n \times n} \). It therefore makes sense to consider the Hessians’ probability space restricted to \( \text{lin}(DS) \), that is considering \( M|_{\text{lin}(DS)} \) and the orthogonal subgroup acting on it, \( O((n-1)^2) \). In this case \( m = (n-1)^2 \). The number of vertices of \( DS \) is the number of permutations which by Stirling’s bound we have \( n! \leq \exp(1 - n + \log n(n + 1/2)) \leq \exp((n-1)^{1.1}) \). Hence the number of edges is bounded by \( \exp(2(n-1)^{1.1}) \), as required.

Lastly, Theorems 3 and 4 can be generalized by considering \( d \)-dimensional faces of the polytope:

**Theorem 5.** If the number of extreme points of the polytope \( \text{hull}(F) \) is bounded by \( \exp(m_{1-r}) \), for some fixed arbitrary \( \epsilon > 0 \), and the Hessian of \( E \) is drawn from the probability space \( (\Omega_m, P_r) \), the chance that a local minimum of \( \min_{X \in \text{hull}(F)} E(X) \) is in the relative interior of a \( d \)-dimensional face of \( \text{hull}(F) \) is extremely small, bounded by \( \exp(-c_1 dm) \), for some constant \( c_1 > 0 \).

This theorem is proved similarly to Theorem 3 by considering indicator variables \( X_\alpha \) for positive semidefinite \( M|_{\text{lin}(\alpha)} \) where \( \alpha \) stands for a \( d \)-dimensional face in \( \text{hull}(F) \). This generalized theorem has a practical implication: local minima are likely to be found on lower dimensional faces.

## 4 Graph matching with one sided permutations

In this section we examine an interesting and popular graph matching (1) instance, where the matchings are the one-sided permutations, namely \( F = \{ X \in \{0,1\}^{r \times n_0} \mid X1 = 1 \} \). That is \( F \) are well-defined maps from graph \( G_A \) with \( n \) vertices to \( G_B \) with \( n_0 \) vertices. This modeling is used in the template and partial matching cases. Unfortunately, in this case, standard graph matching energies \( E(X) \) are not probably conditionally concave over \( \text{lin}(F) \). Note that \( \text{lin}(D_S) \not\subseteq \text{lin}(F) \).

We devise a variation of the Frank-Wolfe algorithm using a *concave search* procedure. That is, in each iteration, instead of standard line search we subtract a convex energy from \( E(X) \) that is constant on \( F \) until we find a descent step. This subtraction is a relaxation of the original problem (1) in the sense it does not alter (up to a global constant) the energy values at \( F \).

The algorithm is summarized in Algorithm 2 and is guaranteed to output a feasible solution in \( F \). The linear program in each iteration over \( \text{hull}(F) \) has a simple closed form solution. Also, note that in the inner loop only \( n \) different \( \lambda \) values should be checked. Details can be found in the supplementary materials.

```
input: X_0 \in \text{lin}(F)
while not converged do
    while energy not reduced do
        add concave energy \( M_{\text{curr}} = M - \lambda \Lambda \):
        compute step: \( X_1 = \min_{X \in \text{lin}(F)} [X_0]^T M_{\text{curr}} [X] \)
        increase \( \lambda \);
    end
    Update current solution \( X_0 = X_1 \) and set \( \lambda = 0 \);
end
```

**Algorithm 2:** Frank-Wolfe with a concave search.
Figure 1: (a) SHREC07 benchmark: Cumulative distribution functions of all errors (left) and mean error per shape (right). (b) Anatomical dataset embedding in the plane. Squares and triangles represent different bone types, lines represent temporal trajectories.

5 Experiments

Bound evaluation: Table 1 evaluates the probability bound (11) for Hessians $M \in \mathbb{R}^{100^2 \times 100^2}$ of $E_2(X)$ using affinities $A, B$ defined by functions of geodesic distances on surfaces. Functions that are conditionally negative definite or semi-definite in the Euclidean case: geodesic distances $d(x, y)$, its square $d(x, y)^2$, and multi-quadratic functions $(1 + d(x, y)^2)^{\gamma}$. Functions that are positive definite in the Euclidean case: $c_{30}([\|x\|]_2) = (1 - \|x\|_2)^+ \frac{1}{2}$, $c_{31}([\|x\|_2]_2) = (1 - \|x\|_2)^+ (4 \|x\|_2 + 1)$ and $\exp(-x^2) \cdot (\|x\|_2^2)$ (note that the last function was used in Vestner et al. (2017)). We also provide the empirical chance of sampling a convex direction. The results in Table 1 are the mean over all the shape pairs (218) in the SHREC07 (Giorgi et al., 2007) shape matching benchmark with $n = 100$. The empirical test was conducted using $10^6$ random directions sampled from an i.i.d. Gaussian distribution. Note that 0 in the table means numerical zero (below machine precision).

Table 1: Evaluation of probable conditional concavity for different functions of geodesics on $\lin(DS)$.

<table>
<thead>
<tr>
<th>Distance</th>
<th>Distance Squared</th>
<th>MultiQuadratic</th>
<th>$c_{30}$</th>
<th>$c_{31}$</th>
<th>Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bound mean</td>
<td>0</td>
<td>0.024</td>
<td>$7 \cdot 10^{-4}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Bound std</td>
<td>0</td>
<td>0.021</td>
<td>$1.7 \cdot 10^{-3}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Empirical mean</td>
<td>0</td>
<td>0.003</td>
<td>$7 \cdot 10^{-5}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Empirical std</td>
<td>0</td>
<td>0.003</td>
<td>$1.8 \cdot 10^{-4}$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Initialization: Motivated by Fischler and Bolles (1987); Kim et al. (2011) and due to the fast running time of the algorithms (e.g., 150msec for $n = 200$ with Algorithm 1 and 16sec with Algorithm 2) both on a single CPU) we sampled multiple initializations based on randomized $l$-pairs of vertices of graphs $G_A, G_B$ and choose the result corresponding to the best energy. In Algorithm 1, we used the Auction algorithm (Bernard et al., 2016), as in Vestner et al. (2017).

Table 2: Comparison to "convex to concave" methods. The table shows the average and the std of the energy differences. Positive averages indicate our algorithm achieves lower energy on average.

<table>
<thead>
<tr>
<th>ModelNet10</th>
<th>SHREC07</th>
</tr>
</thead>
<tbody>
<tr>
<td># points</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>60</td>
</tr>
<tr>
<td>DSPP</td>
<td>5.0±5.3</td>
</tr>
<tr>
<td>PATH</td>
<td>101.4±53.9</td>
</tr>
<tr>
<td>RANDOM</td>
<td>197.9±35.2</td>
</tr>
</tbody>
</table>

Comparison with convex-to-concave methods: Table 2 compares our method to Zaslavskiy et al. (2009); Dym et al. (2017) (PATH, DSPP accordingly). As mentioned in the introduction, these methods solve convex relaxations and then project its minimizer while deforming the energy towards concavity. Our method compares favorably in the task of matching point-clouds from the ModelNet10 dataset (Wu et al., 2015) with Euclidean distances as affinities, and the SHREC07 dataset (Giorgi et al., 2007) with geodesic distances. We used $F = \Pi_n$, and energy (3). The table shows average and standard deviation of energy differences of the listed algorithms and ours; the average is taken over 50 random pairs of shapes. Note that positive averages mean our algorithm achieves lower energy on average; the difference to random energy values is given for scale.
**Automatic shape matching:** We use our Algorithm 1 for automatic shape matching (i.e., with no user input or output shape features) on the SHREC07 (Giorgi et al., 2007) dataset according to the protocol of Kim et al. (2011). This benchmark consists of matching 218 pairs of (often extremely) non-isometric shapes in 11 different classes such as humans, animals, planes, ants etc. On each shape, we sampled $k=8$ points using farthest point sampling and randomized $s=2000$ initializations of subsets of $l=3$ points. In this stage, we use the exact algorithm with initialization using our $n=300$ best result. We then up-sampled to $n=1500$ using the exact algorithm with initialization using our $n=300$ best result. The process takes about 16 min per pair running on a single CPU. Figure 1(a) shows the cumulative distribution function of the geodesic matching errors (left - all errors, right - mean error per pair) of Algorithm 1 with geodesic distances and their functions $c_{30}, c_{31}$. We used (3) and $F = \Pi$. We also show the result of Algorithm 2 with geodesic distances, see details in the supplementary materials. We compare with Blended Intrinsic Maps (BIM) (Kim et al., 2011) and the energies suggested by Boyarski et al. (2017) (heat kernel) and Vestner et al. (2017) (Gaussian of geodesics). For the latter two, we used the same procedure as described above and just replaced the energies with the ones suggested in these works. Note that the Gaussian of geodesics energy of Vestner et al. (2017) falls into the probably concave framework.

**Anatomical shape space analysis:** We match a dataset of 67 mice bone surfaces acquired using micro-CT. The dataset consists of eight time series. Each time series captures the development of one type of bone over time. We use Algorithm 1 to match all pairs in the dataset using Euclidean distance affinity matrices $A, B$, energy (3), and $F = \Pi_n$. After optimization, we calculated a $67 \times 67$ dissimilarity matrix. Dissimilarities are equivalent to our energy over the permutations (up to additive constant) and defined by $\sum_{ijkl} X_{ij} X_{kl} (d_{ik} - d_{jl})^2$. A color-coded matching example can be seen in the inset. In Figure 1(b) we used Multi-Dimensional Scaling (MDS) (Kruskal and Wish, 1978) to assign a 2D coordinate to each surface using the dissimilarity matrix. Each bone is shown as a trajectory. Note how the embedding separated the two types of bones and all bones of the same type are mapped to similar time trajectories. This kind of visualization can help biologists analyze their data and possibly find interesting time periods in which bone growth is changing. Lastly, note that the Tibia bones (on the right) exhibit an interesting change in the midst of its growth. This particular time was also predicted by other means by the biologists.

### 6 Conclusion

In this work, we analyze and generalize the idea of concave relaxations for graph matching problems. We concentrate on conditionally concave and probably conditionally concave energies and demonstrate that they provide useful relaxations in practice. We prove that all local minima of such relaxations are with high probability in the original feasible set; this allows removing the standard post-process projection step in relaxation-based algorithms. Another conclusion is that the set of optimal solutions of such relaxations coincides with the set of optimal solutions of the original graph matching problem.

There are popular edge affinity matrices, such as $\{0, 1\}$ adjacency matrices, that in general do not lead to conditionally concave relaxations. This raises the general question of characterizing more general classes of affinity matrices that furnish (probably) conditionally-concave relaxations. Another interesting future work could try to obtain information on the quality of local minima for more specific classes of graphs.

### 7 Acknowledgments

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