

Isometry pursuit

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Abstract

Isometry pursuit is an algorithm for identifying unitary column-submatrices of wide matrices in polynomial time. It achieves sparsity via use of the group lasso norm, and therefore has constrained and penalized formulations. Applied to tabular data, it selects a subset of columns that maximize diversity. Applied to Jacobians of putative coordinate functions, it identifies isometric embeddings from within dictionaries. It therefore has relevance to interpretability of learned representations.

1 Method

Recall that our objective is to, given a rank D matrix $\mathcal{X} \in \mathbb{R}^{D \times P}$ with $P > D$, select a square submatrix $\mathcal{X}_{\mathcal{S}}$ where subset $\mathcal{S} \subset P$ satisfies $|\mathcal{S}| = D$ that is as unitary as possible. Thus, we first will define a function that is uniquely minimized by unitary matrices and some favorable properties for optimization that will be the ground truth we evaluate the success of our method against. We then define the combination of normalization and multitask basis pursuit that approximates this ground truth loss function. We include claims that ground truth and convex loss values are the same for all diagonalizable matrices, and that the convex basis pursuit program recovers to optimum in a deterministic manner should it exist; proofs are given in Section 2.1. We finally define the lasso dual to the basis pursuit program and a post processing method for ensuring that the solution is D sparse. Experimental results using these methods will then be given in Section ??

1.1 Ground truth

The main goal of isometry pursuit is to expediate the selection of unitary submatrices. More traditional measures of unitariness which use the singular values of a matrix like the log operator norm (i.e. log deformation) and nuclear norm are poorly suited for optimization since they use a subset of the matrix's information and are not uniquely minimized at unitarity, respectively. Thus, we define the loss

$$l_c : \mathbb{R}^{D \times P} \rightarrow \mathbb{R}^+ \quad (1)$$

$$\mathcal{X} \mapsto \sum_{d=1}^D g(\sigma^d(\mathcal{X}), c) \quad (2)$$

where $\sigma^d((X))$ is the d -th singular value of \mathcal{X} and

$$g : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+ \quad (3)$$

$$t, c \mapsto e^{tc} + e^{t^{-c}}. \quad (4)$$

Plainly, g is uniquely maximized by unitary matrices, and $g(\mathcal{X}^\dagger) = g(\mathcal{X})^{-1}$. The former condition is necessary for success of the method, while the latter, as well as the convexity of g , are somewhat aesthetic choices. A graph of g is given in Figure 1. Most importantly, this loss enables comparison with produced after normalization as in Section 1.2.

The overall algorithm we seek to improve upon is

$$\widehat{\mathcal{S}}_{GT} = \arg \min_{\mathcal{S} \subseteq [P]: |\mathcal{S}|=D} l_c(\mathcal{X}_{\mathcal{S}}) \quad (5)$$

In practice, non-convexity occurs in two places, but only one is essential. The inessential non-convexity is in the computation of l_c . While this function is in fact convex, computation of the individual singular values prior to summation is not, and our experiments rely on such piecemeal computation rather than implementing an end-to-end method. However, the combinatorial search over $[P]$ is inherently non-convex, and requires combinatorial search over all combinations.

1.2 Normalization

We will propose a basis pursuit method which approximates the results of Program 5. Since basis pursuit methods tend to select longer vectors, selection of unitary submatrices requires normalization such that long and short candidate basis vectors are penalized in the subsequent regression. This calls for a "normalization" method that differs from other forms in its requirements, and we can't yet prove that these conditions relate it to any sort of norm, even on an appropriately chosen space. This normalization is Now establish some basic conditions for normalization of vectors $v \in \mathbb{R}^D$.

Definition 1 (Symmetric normalization) *A function $q : \mathbb{R}^D \rightarrow \mathbb{R}^+$ is a symmetric normalization if*

$$\arg \max_{v \in \mathbb{R}^D} q(v) = \{v : \|v\| = 1\} \quad (6)$$

$$q(v) = q\left(\frac{v}{\|v\|^2}\right) \quad (7)$$

$$q(v^1) = q(v^2) \quad \forall v^1, v^2 : \|v^1\| = \|v^2\| \quad (8)$$

Note that requiring the full structure of a multiplicative norm here is unnecessary for basic success of the algorithm, but certain characteristics such as $q(v^{-1}) = q(v)$ seem desirable, provided one can give a reasonable way to compute v^{-1} , such as by considering each vector as a scaled rotation subgroup of the general linear group. Mindful of this opportunity, and also of the desire to compare with the ground truth and provide computational expediency, consider the normalization by

$$q : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+ \quad (9)$$

$$t, c \mapsto \frac{e^{t^c} + e^{t^{-c}}}{2e}, \quad (10)$$

and use this to define the vector normalization

$$n : \mathbb{R}^D \times \mathbb{R}^+ \rightarrow \mathbb{R}^D \quad (11)$$

$$n, c \mapsto \frac{n}{q(\|n\|_2, c)} \quad (12)$$

and matrix normalization

$$w : \mathbb{R}^{D \times P} \times \mathbb{R}^+ \rightarrow \mathbb{R}^D \quad (13)$$

$$\mathcal{X}_{.p}, c \mapsto n(\mathcal{X}_{.p}, c) \quad \forall p \in [P]. \quad (14)$$

While this normalization satisfies 1, it also has some additional nice properties. First, q is convex. Second, it grows asymptotically log-linearly. Third, while $\exp(-|\log t|) = \exp(-\max(t, 1/t))$ is a seemingly natural choice for normalization, it is non smooth, and the LogSumExp replacement of $\max(t, 1/t)$ with $\log(\exp(t) + \exp(1/t))$ simplifies to 9 upon exponentiation. Finally, the parameter c grants control over the width of the basin, which is important in avoiding numerical issues arising close to 0 and ∞ . This completes the deterministic data preprocessing.

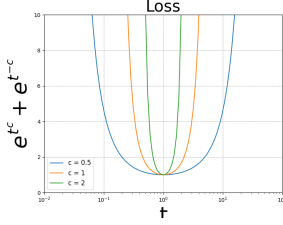


Figure 1: Ground truth loss scaling function g as a function of t

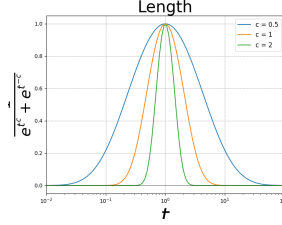


Figure 2: Length as a function of t

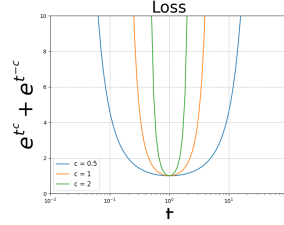


Figure 3: Basis pursuit losses as a function of t

Figure 4: Plots of Length and Loss for different values of c . Since t is one dimensional and therefore diagonalizable, basis pursuit and ground truth give identical loss values.

1.3 Isometry pursuit

We will show how to use an appropriate normalized matrix $w(\mathcal{X})$ in multitask basis pursuit to identify submatrices of \mathcal{X} that are as unitary as possible. Multitask basis pursuit is a method for identifying sparse signals from overcomplete dictionaries, and the intuition behind its application in our setting is that submatrices consisting of vectors which are closer to 1 in length and more orthogonal will have smaller loss. In contrast to the typical statistical setting, these features correspond to individual observations in our diversification example, and basis vectors of data manifold tangent spaces in our non-linear dimension reduction example.

Define the multitask basis pursuit penalty

$$\|\cdot\|_{1,2} : \mathbb{R}^{P \times D} \rightarrow \mathbb{R}^+ \quad (15)$$

$$\beta \mapsto \sum_{p=1}^P \|\beta_p\|_2. \quad (16)$$

The isometry pursuit program is then

$$\hat{\beta}_c^D(\mathcal{X}) := \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta\|_{1,2} : I_D = w(\mathcal{X}, c)\beta. \quad (17)$$

The recovered functions are the indices of the dictionary elements with non-zero coefficients. That is, they are given by $S(\beta)$ where

$$S : \mathbb{R}^{p \times d} \rightarrow \binom{[P]}{d} \quad (18)$$

$$\beta \mapsto \{p \in [P] : \|\beta_p\| > 0\} \quad (19)$$

and $\binom{[P]}{d} = \{A \subseteq [P] : |A| = d\}$.

ISOMETRYPURSUIT(Matrix $\mathcal{X} \in \mathbb{R}^{D \times P}$, scaling constant c)

1: **Output** $\hat{S} = S(\hat{\beta}_P(w_c(\mathcal{X})))$

A key theoretical assertion for the feasibility of ISOMETRYPURSUIT is that it is invariant to choice of basis for \mathcal{X} .

Proposition 1 (Basis pursuit selection invariance) *Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $S(\hat{\beta}(U\mathcal{X})) = S(\hat{\beta}(\mathcal{X}))$.*

A proof is given in Section 2.1.1 This fact has as an immediate corollary that we may replace I_D in the constraint by any unitary $D \times D$ matrix.

With these preliminaries, we may state our main result. From an intuitive perspective, this is akin to saying selected columns are not only complementary in that they are orthogonal, but also well-balanced in that their columns are of a length 1 rather than length 0.

Proposition 2 (Unitary selection) *Given a matrix $\mathcal{X} \in \mathbb{R}^{D \times P}$ with a rank D submatrix $\mathcal{X}_S \in \mathbb{R}^{D \times D}$ that is the unique $D \times D$ rank D -unitary submatrix, $S = S(\hat{\beta}_c^P(\mathcal{X})) \forall c \in \mathbb{R}^+$.*

This proof admits two immediate generalizations. First, any normalization function that satisfies the normalization conditions will do. Second, assuming that we do in fact use w for normalization, the ground truth and convex losses are equivalent for diagonalizable matrices. This is summarized in the following proposition, which is slightly stronger than Proposition 2

Proposition 3 (Loss equivalence) *Given a diagonalizable matrix $\mathcal{X} \in \mathbb{R}^{D \times D}$, $\|\hat{\beta}_c^P(\mathcal{X})\|_{1,2} = l_c(\mathcal{X})$.*

This proposition should be thought of as applying to D column matrices after selection. We know that unitary submatrices minimize loss, and should they be present, they will be selected by either method. This proposition shows that should diagonalizable matrices be selected, they will also have equivalent loss, but not necessarily that they will be selected.

1.4 Isometric lasso

The convex loss function 15 and linear constraint in 17 admit a Lagrangian dual which we shall call Isometric Lasso. While we defer full discussion of computational complexity to Section ??, the general principal which motivates the use of this formulation in our setting is the increased computational expediency in high-dimensions.

The Isometric Lasso loss is

$$l_\lambda(\mathcal{X}, \beta) = \|I_D - \tilde{\mathcal{X}}_c \beta\|_2^2 + \lambda \|\beta\|_{1,2} \quad (20)$$

which can be optimized as

$$\hat{\beta}_\lambda(\mathcal{X}) = \arg \min_{\beta \in \mathbb{R}^{P \times D}} l_\lambda(\mathcal{X}, \beta) \quad (21)$$

Similarly to Section ??, we assert that $S(\hat{\beta}_\lambda(\mathcal{X}))$.

Proposition 4 (Lasso selection equivalence) *Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $S(\hat{\beta}_\lambda(U\mathcal{X})) = S(\hat{\beta}_\lambda(\mathcal{X}))$.*

This also covers changing the target variable.

Note that it also may be possible to argue the basis pursuit invariance from the lasso ones plus Lagrangian duality, but to avoid taking the limit we prove both propositions independently.

1.5 Extension to non-linear spaces

Proposition 5 (Isometry at a point selection) *Given a set of functions G that contains a subset that defines a locally isometric embedding at a point ξ , then these will be selected as $\arg \min_\beta$.*

A proof is given in Section 2.1.2.

1.6 Two-stage isometry pursuit

A standard approach in the lasso literature is to first use the lasso to prune, prior to a final feature selection step **Hesterberg2008-iy** This avoids issues from shrinkage caused by the lasso estimator at high values of λ . For example, we cannot as of yet prove analogs of Proposition 2 for the Lasso formulation, and similar lasso-specific conditions such as those found in **Koelle2024-no** are not satisfied by overcomplete dictionaries.

1.7 Implementation

We use the multitask lasso from sklearn and the cvxpy package for basis pursuit. We use the SCS interior point solver from CVXPY, which is able to push sparse values arbitrarily close to 0 **cvxpy'sparse'solution**. Data is IRIS and Wine, as well as flat torus from ldle.

1.8 Computational complexity

2 Supplement

We give proofs in support of the propositions in the main text and supplemental experimental information to better contextualize the results.

2.1 Proofs

2.1.1 Proof of Proposition 1

In this proof we first show that the penalty $\|\beta\|_{1,2}$ is unchanged by unitary transformation of β .

Proposition 6 *Loss equivalence* Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $\|\beta\|_{1,2} = \|\beta U\|$.

Proof:

$$\|\beta U\|_{1,2} = \sum_{p=1}^P \|\beta_p U\| \quad (22)$$

$$= \sum_{p=1}^P \|\beta_p\| \quad (23)$$

$$= \|\beta\|_{1,2} \quad (24)$$

□

We then show that this implies that the resultant loss is unchanged by unitary transformation of \mathcal{X} .

Proposition 7 Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $\hat{\beta}(U\mathcal{X}) = \hat{\beta}(\mathcal{X})U$.

Proof:

$$\hat{\beta}(U\mathcal{X}) = \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta\|_{1,2} : I_D = UX\beta \quad (25)$$

$$= \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta\|_{1,2} : U^{-1}U = U^{-1}UX\beta U \quad (26)$$

$$= \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta\|_{1,2} : I_D = X\beta U \quad (27)$$

$$= \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta U\|_{1,2} : I_D = X\beta U \quad (28)$$

$$= \arg \min_{\beta \in \mathbb{R}^{P \times D}} \|\beta\|_{1,2} : I_D = X\beta. \quad (29)$$

□

2.1.2 Proof of Proposition 2

In support of the proposition in the main text, we give a more general theorem which illustrates the key features of the method. From there, it is a straightforward step to specify to the chosen normalization.

First, we state the more general version of Proposition ??.

Proposition 8 (Generalized unitary selection) *Given a matrix $\mathcal{X} \in \mathbb{R}^{D \times P}$ with a rank D submatrix $\mathcal{X}_{\mathcal{S}} \in \mathbb{R}^{D \times D}$ that is the unique $D \times D$ rank D -unitary submatrix, and let n_q be a normalization composed of normalizing functions q that satisfy the conditions of Definition ??, then conditions $\mathcal{S} = \mathcal{S}(\hat{\beta}_q^P(\mathcal{X}))$.*

Proof: The first component of this proof deals with D -sparse solutions only. In this section, there are two main claims: that, given that a matrix consists of column-vectors of a certain set of lengths, loss will be minimized if these vectors are orthogonal, and that, given that a matrix consists of orthogonal columns, loss will be minimized if these vectors are of length one. These propositions suffice to show that, of all D -sparse solutions, the minimizer will be the unique unitary submatrix. The second step of the proof consists of the claim that D -sparse solutions are preferable to those consisting of more components. We proceed similarly, showing that loss is reduced by making any D -column submatrix of the putative solution orthonormal, and that loss is minimized further by removal of the non orthonormal components. \square

Proposition 9 *Let $X \in \mathbb{R}^{D \times P}$. Also, let X have a submatrix $\tilde{X}_{\mathcal{S}} \in \mathbb{R}^{D \times D}$ such that $\|\tilde{X}_{\mathcal{S}}^{S_p}\|_2 = \|X_{\mathcal{S}}^{S_p}\|_2$ for all $j \in [d]$ and $X_{S_p} X^{S_p} = \begin{cases} 1 & : p_1 = p_2 \\ 0 & : p_1 \neq p_2 \end{cases}$. Let this be the only such D submatrix of X . Then $l(X_{\mathcal{S}}) < l(X_{\mathcal{S}'})$.*

Proof: By Lemma 7, without loss of generality

$$\beta_{jk}^i = \begin{cases} \|\tilde{X}'_{\mathcal{S}_j}\|_2^{-1} & j = k \in \{1 \dots d\} \\ 0 & \text{otherwise} \end{cases}. \quad (30)$$

Therefore,

$$\tilde{l}^*(X') = \sum_{j=1}^d \sqrt{\sum_{i=1}^n \|\tilde{X}'_{i,\mathcal{S}_j}\|_2^{-2}}. \quad (31)$$

On the other hand, the invertible matrices $\tilde{X}_{\mathcal{S}}$ admit QR decompositions $\tilde{X}_{\mathcal{S}} = QR$ where Q and R are square unitary and upper-triangular matrices,

respectively **Anderson1992-fb**. Since l^* is invariant to unitary transformations, we can without loss of generality, consider $Q = I_d$. Denoting I_d to be composed of basis vectors $[e^1 \dots e^d]$, the matrix R has form

$$R = \begin{bmatrix} \langle e^1, \tilde{X}_{i.S_1} \rangle & \langle e^1, \tilde{X}_{i.S_2} \rangle & \dots & \langle e^1, \tilde{X}_{i.S_d} \rangle \\ 0 & \langle e^2, \tilde{X}_{i.S_2} \rangle & \dots & \langle e^2, \tilde{X}_{i.S_d} \rangle \\ 0 & 0 & \dots & \dots \\ 0 & 0 & 0 & \langle e^d, \tilde{X}_{i.S_d} \rangle \end{bmatrix}. \quad (32)$$

The diagonal entries $R_{jj} = \langle q^j, \tilde{X}_{i.S_j} \rangle$ of this matrix have form $\|\tilde{X}_{i.S_j} - \sum_{j' \in \{1 \dots j-1\}} \langle \tilde{X}_{i.S_j}, e^{j'} \rangle e^{j'}\|$. Thus, $R_j \in (0, \|\tilde{X}_{i.S_j}\|]$. On the other hand $\beta_{i.S} = R^{-1}$, which has diagonal elements $\beta_j = R_j^{-1}$, since R is upper triangular. Thus, $\beta_{jj} \geq \|\tilde{X}_{i.S_j}\|^{-1}$, and therefore $\|\beta_{i.S_j}\| \geq \|\beta'_{S_j}\|$. Since $\|\beta_{S_j}\| \geq \|\beta'_{S_j}\|$ for all i , then $\|\beta_{S_j}\| \geq \|\beta'_{S_j}\|$. \square

The above proposition formalizes our intuition that orthogonality of X lowers $l^*(X)$ over non-orthogonality.

Since vectors which are closer to length 1 are shrunk in length less by \exp_1 , their corresponding loadings are smaller. This is formalized in the following proposition

Proposition 10 *Let $X''_{.S}$ be a set of vector fields $X''_{.S_j}$ mutually orthogonal at every data point i , and $\|X''_{.S_j}\| = 1$. Then $\tilde{l}^*(X'_{.S}) \geq \tilde{l}^*(X''_{.S})$.*

Proof: Let $\|X''_{i.S_j}\| = c_j$. By Proposition ??, we can assume without loss of generality (i.e without changing the loss) that

$$\tilde{X}_{i.S_j} = \begin{bmatrix} c_1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & c_d \end{bmatrix}. \quad (33)$$

Thus

$$\exp_1 X_{i.S_j} = \begin{bmatrix} \exp(-|\log \|c_1\|_2|) & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & \exp(-|\log \|c_d\|_2|) \end{bmatrix}. \quad (34)$$

and therefore

$$\tilde{\beta}_{i.S_j} = \begin{bmatrix} \exp(-|\log \|c_1\|_2|)^{-1} & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & \exp(-|\log \|c_d\|_2|)^{-1} \end{bmatrix}. \quad (35)$$

The question is therefore what values of c_j minimize $\exp(-|\log \|c_1\|_2|)^{-1}$. $|\log \|c_1\|_2|$ is minimized (evaluates to 0) when $c_j = 1$, so $-\log \|c_1\|_2|$ is maximized (evaluates to 0, so $\exp(-|\log \|c_1\|_2|)$ is maximized (evaluates to 1), so $\exp(-|\log \|c_1\|_2|)^{-1}$ is minimized (evaluates to 1). \square

Proposition 11 (Support contraction) *Let X and S' be solutions such that in X' a submatrix $X_{.S}$ orthonormalized. That is, $X_{.S}^T X_{.S} = I_D$ while $X_p = X'_{.p} \forall p \notin S$. Then $l(X') \leq l(X)$.*

Proof: Since X' is full rank, there exists $\gamma_{Sc} : X'_{.S} \gamma_{Sc} = X_c$ for $c \notin S$. Then $X_c \beta = X'_{.S} \gamma_{Sc} \beta$. Then $I_D - X_S \beta_S =$ \square

2.1.3 Proof of Proposition 4

This proof proceeds similarly to the proof of Proposition ?? . Proposition 4 relies on the fact that its loss is invariant under any unitary transformation. As a corollary, this fact gives that the identify matrix which is the "dependent variable" in the regression equation may be replaced by any $d \times d$ unitary matrix. For Proposition ??, the loss is also invariant under unitary, transformation, but we also check that this transformation. Once again, this also implies that any unitary matrix may replace the identity in the constraint.

Proposition 12 Loss equivalence *Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $l_\lambda(\mathcal{X}, \beta) = l_\lambda(U\mathcal{X}, \beta U)$.*

Proof: Without loss of generality, let $i = 1$. We can write

$$l^*(X^i) = l(\beta^i) = \sum_{j=1}^p \left(\sum_{i'=2}^n \|\beta_{i'j}\|_2^2 + \|\beta_{1j}^i\|_2^2 \right)^{1/2} = \sum_{j=1}^p \left(\sum_{i'=1}^n \|\beta_{i'j} U\|_2^2 \right)^{1/2} = l^*(X) \quad (36)$$

where the second to last equality is because the norm $\|v\|_2^2$ is unitary invariant. \square

Proposition 13 Programmatic equivalence *Let $U \in \mathbb{R}^{D \times D}$ be unitary. Then $\hat{\beta}_\lambda(U\mathcal{X}) = U \hat{\beta}_\lambda(\mathcal{X})$.*

2.2 Experiments