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Invariants of gradient (Morse) complexes and artificial neural nets

Serguei Barannikov

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Abstract

There is canonical partition of set of critical values of smooth function into pairs "birth-death" and a separate set representing basis in Betti homology, as was established in S.Barannikov "The Framed Morse complex and its invariants" Adv. in Sov. Math., vol 21, AMS transl, (1994). This partition arises from bringing the gradient (Morse) complex to so called "canonical form" by a linear transform respecting the filtration defined by the order of the critical values. These "canonical forms" are combinatorial invariants of $\mathbb{R}-$ filtered complexes. Starting from the beginning of 2000s these invariants became widely used in applied mathematics under the name of "Persistence diagrams" and "Persistence Bar-codes". The canonical form of an $\mathbb{R}-$ filtered complex is the partition of the set of critical values (indices of filtration) into "birth-death" pairs and a separate set representing homology of the complex. The "canonical form" invariants are obtained by action of upper-triangular matrices, which reduces the $\mathbb{R}-$ filtered complex to the simplest form. In this note I give a short introduction into the subject of these invariants. I also propose application of these invariants to artificial neural nets.

Notations.

Let F denotes a field, in most our examples below $F = \mathbb{R}$ the field of real numbers.

1 Chain complexes.

Recall that a chain complex (C_*, ∂_*) is a sequence of vector spaces over field F and linear operators

$$\to C_{j+1} \stackrel{\partial_{j+1}}{\to} C_j \stackrel{\partial_j}{\to} C_{j-1} \to \ldots \to C_0$$

which satisfy

$$\partial_j \circ \partial_{j+1} = 0$$

The $j-$ th homology of the chain complex (C_*, ∂_*) is the quotient

$$H_j = \ker(\partial_j) / \mathrm{im}(\partial_{j+1}).$$

1.1 Morse complex

Let $f : M^n \to \mathbb{R}$, $f \in C^\infty$, is a generic function such that its sublevel sets $\{x \mid f(x) \le c\}$ are compact. Then the critical points p_α, $df\,|_{T_{p_\alpha}} = 0$, are isolated, and near such p_α the function can be written as $f = \sum_{l=1}^{j} -(x^l)^2 + \sum_{l=j}^{n} (x^l)^2$. Let g be a generic metric. Then define

$$C_j = \oplus_{\mathrm{index}(p_\alpha)=j} \left[p_\alpha, \mathrm{or}(T^-_{p_\alpha})\right]$$

where $T_{p_\alpha} = T^-_{p_\alpha} \oplus T^+_{p_\alpha}$ is decomposed with respect to the quadratic forms $\partial^2 f$ and g.

The differential is defined as

$$\partial_j\,[p_\alpha, \mathrm{or}] = \sum_{\mathrm{index}(p_\beta)=j-1} [p_\beta, or]\,\#\mathcal{M}(p_\alpha, p_\beta)$$

where $\#\mathcal{M}(p_\alpha, p_\beta)$ is the number of trajectories

$$\mathcal{M}(p_\alpha, p_\beta) = \left\{\gamma : \mathbb{R} \to M^n \mid \dot\gamma = -(\mathrm{grad}_g f)(\gamma(t)), \lim_{t\to-\infty} = p_\alpha, \lim_{t\to+\infty} = p_\beta\right\}/\mathbb{R}$$

counted with sign given by the ratio of the orientation $\mathrm{or}(T^-_{p_\alpha})$ transported along the trajectory and $\mathrm{or}(T^-_{p_\beta}) \otimes \lim_{t\to+\infty}\gamma(t)_*\mathrm{or}(\mathbb{R})$.

The differential satisfies $\partial_j \circ \partial_{j+1} = 0$. It follows from considering the boundary of $1-$ dimensional families $\mathcal{M}(p_\alpha, p_\lambda)$ with $\mathrm{index}(p_\lambda) = \mathrm{index}(p_\alpha) - 2$, see [B94] and references therein.

2 Canonical forms (=persistence diagrams/barcodes) of $\mathbb{R}-$ filtered chain complexes.

Let C_* is an $\mathbb{R}-$ filtered chain complex, an increasing sequence of subcomplexes $F_sC_* \subset F_rC_*$, $s < r$, indexed by finite set of real numbers, $F_{max}C_* = C_*$. It can come with a basis compatible with filtration so that each subspace F_rC_j is the span $\left\langle e_1^{(j)}, \dots, e_{i_r}^{(j)}\right\rangle$.

Let C_* , $\{e_i^{(j)}\}_{j\in\{0,1,\dots\}}^{i\in 1,\dots,\dim_F C_j}$ be a chain complex together with bases in C_j .Consider arbitrary *upper-triangular* changes of bases in C_j .

Definition 2.1. Let us call a chain complex $\tilde C_*$ with ordered bases $\{\tilde e_i^{(j)}\}_{j\in\{0,1,\dots\}}^{i\in 1,\dots,\dim_F C_j}$ a complex in "canonical form" if

1. For any basis element $\tilde e_i^{(j)}$ either $\partial\tilde e_i^{(j)} = 0$ or $\partial\tilde e_i^{(j)} = \tilde e_{i'}^{(j-1)}$.
2. In the latter case, for two different basis elements $\tilde e_{i_1}^{(j)} \neq \tilde e_{i_2}^{(j)} \Rightarrow \partial\tilde e_{i_1}^{(j)} \neq \partial\tilde e_{i_2}^{(j)}$.

Theorem 2.2. *([B94]) An $\mathbb{R}-$ filtered chain complex C_* with bases $\{e_i^{(j)}\}_{j\in\{0,1,\dots\}}^{i\in 1,\dots,\dim_F C_j}$ compatible with the filtration can be reduced by <u>upper-triangular</u> changes of bases $A^{(j)} \in GL\,(C_j)$*

$$A^{(j)} = \begin{pmatrix} f_{11} & f_{12} & \dots & f_{1k} \\ 0 & f_{22} & & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & f_{kk} \end{pmatrix}$$

to a complex in the "canonical form". This complex in the "canonical form" is determined uniquely by the original $\mathbb{R}-$ filtered complex .

Proof. For reader convenience we reproduce here the proof from §2,[B94]. Suppose that for $p = j$ and $m \le i$, or $p < j$ and all m , $\partial e_m^{(p)}$ has the required form. I.e. either $\partial e_m^{(p)} = 0$, or $\partial e_m^{(p)} = e_{l(m)}^{(p-1)}$, where $l(m) \neq l(m')$ for $m \neq m'$. Let's simplify $\partial e_{i+1}^{(j)}$. Let

$$\partial e_{i+1}^{(j)} = \sum_k e_k^{(j-1)}\alpha_k. \tag{1}$$

Let's move all the terms with $e_k^{(j-1)} = \partial e_q^j$, $q \le i$, from the right to the left in (1). I get

$$\partial(e_{i+1}^{(j)} - \sum_{q\le i} e_q^{(j)}\alpha_{k(q)}) = \sum_k e_k^{(j-1)}\beta_k$$

If $\beta_k = 0$ for all k, then define $\tilde{e}^{(j)}_{i+1} = e^{(j)}_{i+1} - \sum_{q\le i} e^{(j)}_q \alpha_{k(q)}$. Then $\partial \tilde{e}^{(j)}_{i+1} = 0$ and for $m \le i$ and $p = j$ and, or $p < j$ and all m, $\partial e^{(p)}_m$ continues to have the required form. Otherwise let k_0 be the maximal k with $\beta_k \neq 0$. Then

$$\partial(e^{(j)}_{i+1} - \sum_{q\le i} e^{(j)}_q \alpha_{k(q)}) = e^{(j-1)}_{k_0}\beta_{k_0} + \sum_{k<k_0} e^{(j-1)}_k \beta_k,\ \beta_{k_0} \neq 0.$$

where $k_0 \neq k(q)$ for $q \le i$. Since $\partial e^{(j-1)}_m$ has the required form for all m, it follows that $\partial e^{(j-1)}_k = 0$ for any k such that $\beta_k \neq 0$. Define

$$\tilde{e}^{(j)}_{i+1} = \left(e^{(j)}_{i+1} - \sum_{q\le i} e^{(j)}_q \alpha_{k(q)}\right)/\beta_{k_0},\ \tilde{e}^{(j-1)}_{k_0} = e^{(j-1)}_{k_0} + \sum_{k<k_0} e^{(j-1)}_k \beta_k/\beta_{k_0}.$$

Then $\partial \tilde{e}^{(j)}_{i+1} = \tilde{e}^{(j-1)}_{k_0}$ and for $p = j$ and $m \le i$, or $p < j$ and all m, $\partial e^{(p)}_m$ continues to have the required form. If the complex has been reduced to canonical form up to index j, then reduce similarly the expression for $\partial e^{(j+1)}_1$ and so on.

Let us prove the uniqueness of the canonical form of C_* over F. It follows essentually from the uniqueness at each step of the described algorithm for calculation of canonical form. Let $\left\{a^{(j)}_i\right\}$, $\left\{b^{(j)}_i\right\}$ be two ordered bases of C_* for the two canonical forms. Assume that for all indexes $p < j$ and all n, and $p = j$ and $n \le i$ the canonical forms agree, i.e. if $da^{(p)}_n = a^{(p-1)}_k$ then $\partial b^{(p)}_n = b^{(p-1)}_k$, or similarly if $\partial a^{(p)}_n = 0$ then $\partial b^{(p)}_n = 0$. Let $\partial a^{(j)}_{i+1} = a^{(j-1)}_m$ and $\partial b^{(j)}_{i+1} = b^{(j-1)}_l$ with $m > l$. Note that

$$b^{(j)}_{i+1} = \sum_{k\le i+1} a^{(j)}_k \alpha_k,\ b^{(j-1)}_l = \sum_{n\le l} a^{(j-1)}_n \beta_n$$

where $\alpha_{i+1} \neq 0$, $\beta_l \neq 0$. Hence

$$\partial\left(\sum_{k\le i+1} a^{(j)}_k \alpha_k\right) = \sum_{n\le l} a^{(j-1)}_n \beta_n,$$

or $\partial\left(\sum_{k\le i+1} a^{(j)}_k \alpha_k\right) = 0$. Therefore

$$\partial a^{(j)}_{i+1} = \sum_{n\le l} a^{(j-1)}_n \beta_n/\alpha_{i+1} - \sum_{k\le i} \partial a^{(j)}_k \alpha_k/\alpha_{i+1}$$

On the other hand $\partial a^{(j)}_{i+1} = a^{(j-1)}_m$, with $m > l$, and $\partial a^{(j)}_k$ for $k \le i$ are either zero or some basis elements different from $a^{(j-1)}_m$. This gives a contradiction and the canonical forms agree for $p = j$ and $n = i+1$. Similarly if $\partial a^{(j)}_{i+1} = a^{(j-1)}_m$ and $\partial b^{(j)}_{i+1} = 0$, then, analogously, $\partial\left(\sum_{k\le i+1} a^{(j)}_k \alpha_k\right) = 0$, where $\alpha_{i+1} \neq 0$, $\partial a^{(j)}_{i+1} = -\sum_{k\le i} \partial a^{(j)}_k \alpha_k/\alpha_{i+1}$ and, since $\partial a^{(j)}_k$ for $k \le i$ are either zero or some basis elements different from $a^{(j-1)}_m$ this gives again a contradiction. This proves the uniqueness of the canonical form of C_* over F. □

Remark 2.3. The "canonical form" of an $\mathbb{R}-$ filtered complex can be described as the partition of the set of real numbers which are indexes of the filtration into pairs "birth"-"death" plus a separate set of indexes representing basis in homology. In many natural cases the critical values are the natural indexes and this theorem gives such canonical decomposition of the set of crtitical values into pairs "birth"-"death" plus a separate set of critical values ("spectral invariants") representing a basis in homology.

2.1 "Canonical form" invariants of Morse complexes.

Consider the complex $C_*(f,g)$ associated with a Morse function f and its gradient flow with respect to metric g. The basis elements, given by critical points in each C_i are naturally ordered by the heights of the critical values. For generic function the critical values are all distinct. So the complex $C_*(f,g)$ is a chain complex with ordered bases.

Theorem 2.4. *([B94]) The canonical form of the Morse complex $C_*(f,g)$ with ordered generators is invariant with respect to change of the metrics.*

Proof. The only metamorphoses of the complex $C_*(f, g_t)$ in a generic 1-parameter family of metrics g_t arise when there is an anti-gradient trajectory leading from a critical point $e_i^{(j)}$ to a critical point $e_k^{(j)}$ of the same index and with *lower* critical value. The change of the complex under such metamorphosis is described by the change of the basis given by elementary *upper-triangular* matrix: $\tilde{e}_i^{(j)} = e_i^{(j)} + e_k^{(j)}$. Now the invariance follows from the uniqueness of the "canonical form" of the complex with ordered generators. □

2.2 Classification and structure theorems for $\mathbb{R}-$ filtered complexes.

The theorem 2.2 gives also the classification and the structure theorems for $\mathbb{R}-$ filtered chain complexes:

Corollary 2.5. *(Classification) Two $\mathbb{R}-$ filtered chain complexes are isomorphic if and only if their "canonical form" invariants coincide.*

Corollary 2.6. *(Structure theorem) The category of $\mathbb{R}-$ filtered chain complexes is semi-simple: any $\mathbb{R}-$ filtered chain filtered complex over a field F can be brought by a linear transformation preserving the filtration to "canonical form", a canonically defined direct sum of $\mathbb{R}-$ filtered complexes of two types: one-dimensional complexes with trivial differential $d(e_{t_i}) = 0$ and two-dimensional complexes with trivial homology $d(e_{s_j}) = e_{r_j}$.*

2.3 Algorithm.

The proof of the theorem 2.2 from (§2.1, [B94]) is constructive and contains the algorithm for calculation of the "canonical form".

Corollary 2.7. *The algorithm for calculation of the "canonical form" invariant was described in (§2.1, [B94]). The algorithm takes as input an $\mathbb{R}-$ filtered chain complex and gives as output its "canonical form", a canonically defined direct sum of filtered complexes of two types: one-dimensional complexes with trivial differential $d(e_{t_i}) = 0$ and two-dimensional complexes with trivial homology $d(e_{s_j}) = e_{r_j}$. It acts via the action by upper-triangular matrices.*

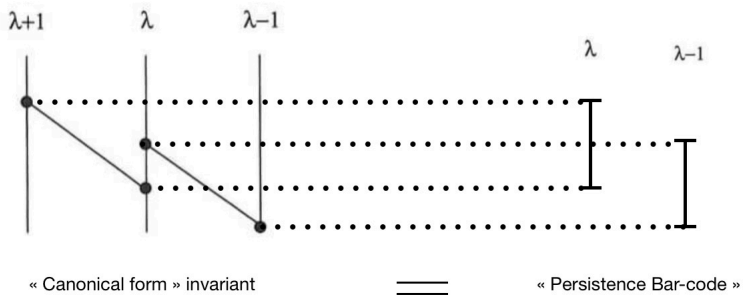
2.4 Deformations and stability of the canonical form.

Corollary 2.8. *(Stability). Under continuous deformation of the filtration the canonical form is changed by the natural shifting of the indices of the filtration for each one-dimensional complexes with trivial differential $d(e_{t_i}) = 0$ and two-dimensional complexes with trivial homology $d(e_{s_j}) = e_{r_j}$, and by removing or/and adding a two-dimensional complexes with trivial homology $d(e_{s_j}) = e_{r_j}$ on the same level: $r_j = s_j$.*

It is straightforward then to express this stability stattement in $\varepsilon - \delta$ language.

2.5 Comparison with "persistence diagrams" or "persistence bar-codes".

There are three equivalent visualizations of the same invariants. "Persistence Bar-codes"/"Persistence diagrams" were introduced in the beginning of 2000s (H.Edelsbrunner, J.Harer, A.Zamorodian "Hierarchical Morse complexes for piecewise linear 2-manifolds" Proc. of Symp on Comput Geometry, June 2001).



There are more than ten software packages for computing these invariants of a finite filtration. The principal algorithm is based on the bringing of the filtered complex to its canonical form by upper-triangular matrices from (§2.1, [B94]).

3 The invariants $d(p_i)$ of local minima.

I give in this section three equivalent definitions of the invariants $d(p_i) \in \mathbb{R}_{>0}$ attached to local minima p_i .

3.1 Pairs "minimum - saddle point of index 1" in the canonical form.

The $0-$ th homology of the gradient (Morse) complex of l are $1-$ dimensional. Each local minimum p_i which is not global is paired in the canonical form with an index 1 saddle point q_i of "death" type:

$$p_i \leftrightarrow q_i.$$

The invariant $d(p_i) \in \mathbb{R}_{>0}$ of the local minimum p_i is by definition the difference of the critical values

$$d(p_i) = l(q_i) - l(p_i).$$

3.2 New global minimum on one of connected component of $\{x \mid l(x) \leq l(q_i) - \epsilon\}$.

If q_i is a saddle point of the "death" type then the number of connected components of the set $\{x \mid l(x) \leq l(q_i) - \epsilon\}$ is equal to the number of connected components of the set $\{x \mid l(x) \leq l(q_i) + \epsilon\}$ increased by 1 . The restriction of l to each connected component has its global minimum. The minimum p_i paired with q_i is the *new* global minimum of the restriction of l to one of the connected component of the set $\{x \mid l(x) \leq l(q_i) - \epsilon\}$.

3.3 The lowest saddle on a way to a lower minima.

The index 1 saddle q_i paired with a local minimum p_i is the lowest saddle which belongs to a 1-parameter path connecting p_i with a lower local minimum. In other words $d(p_i)$ is the minimal height which must be climbed from the local minimum p_i in a 1-parameter path from p_i to a lower local minimum.

4 Characterisation of generalisability and trainability of artificial neural nets via the invariants $d(p_i)$ of local minima of loss.

I propose the following characterisation of generalisability of the neural net. In the previuos section I have associated with each local minimum p_i the positive real number $d\,(p_i)$. The *generalisability* of the neural net is good if and only if for any local minimum p_i with low $l(p_i)$ the invariant $d\,(p_i)$ is small:

$$(l(p_i) - l_{\min}) \text{ is small} \Rightarrow d\,(p_i) \text{ is small}$$

Arbitrary local minima with big value of $d(p_i)$ affect trainability of the neural net. The bigger $d(p_i)$ at some local minima p_i is, the higher are the chances that the trajectory of gradient descent may get stucked at p_i.

5 Calculation of the invariants $d(p_i)$ of local minima via "1-parameter gradient descent".

To find local minima of the loss function in situations when number of parameters is very big the gradient descent is applied successfully. A kind of "1-parameter gradient descent" can be applied in this situation to determine the invariants $d(p_i)$ of local minima. Each index 1 saddle point has two descending anti-gradient trajectories going to two local minima. Let $s(t)$ be a path between two local minima p and p'. The curve is deformed by the vector field $-\mathrm{grad}\, l$. Namely apply the modified gradient descent with respect to $-\mathrm{grad}_n l(t)$, the normal component of $-\mathrm{grad}\, l$ at $s(t)$, to $s(t)$, or more precisely to a set of points approximating $s(t)$. The maximum value of the loss function on the curve

$$l_{\max}(s) = \max_t l(s(t))$$

decreases in each iteration. In the simplest case the curve converges to a curve $s_{\lim}(t)$ passing through one index-one saddle point and consisting of two anti-gradient trajectories each going from the saddle to one of two minima. In general the curve converges to a curve $s_{\lim}(t)$ passing through j index-one saddle points and consisting of $2j$ anti-gradient trajectories each going from one of the index-one saddles to one of several minima. The saddles correspond to local maxima of the loss function on the limiting curve. The maximum of the loss l on such limiting curves connecting p with a lower minimum p' minus $l(p)$ is the invariant $d(p)$:

$$\max_{p':l(p')<l(p)} \left(\max_t l(s_{lim}(t))\right) - l(p) = d(p)$$

6 Behaviour of the invariants $d(p_i)$ under adding of extra layer.

Proposition 6.1. *The invariants $d(p_i)$ of the loss function of the neural nets decrease with adding of an extra layer.*

Proof. It follows from the fact that the loss as function of the added weights and biases of the extra layer is picewise quadratic and everywhere nonnegative. □

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