Supporting Information

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SI Text: Additional Background on Scales of Phenotypic Integration, Further Analysis of Modularity in *Smilodon fatalis*, and Additional Methods

Scales of Phenotypic Integration and Modularity. Studies of phenotypic integration and modularity can focus on several scales and different causal mechanisms. The most commonly used approach, termed variational integration (1, 2), focuses on population- or species-level patterns, typically derived from a large sample of adult specimens. Unless qualified as one of the following more specific levels, the terms phenotypic integration and modularity here refer to this variational scale. One can further focus on developmental integration (covariation among traits driven by shared developmental processes), functional integration (covariation driven by coordination for a shared or linked function), genetic integration (covariation driven by pleiotropic effects), environmental integration (covariation driven by similar phenotypic plasticity of traits in response to environmental variation), or ontogenetic integration (covariation driven by coordination through development, often analyzed with a comparative sample across ontogenetic stages) (2). Perhaps most important from a deep-time perspective is the study of evolutionary integration and its counterpart evolutionary modularity, in which analyses may sample widely across phylogeny or through geologic time to identify shifts in trait integration. Each of these scales and foci for studying phenotypic integration has methodological complexities, in many cases related to the quality and heterogeneity of the available sample, and several recent reviews discuss these issues in detail (2–4). Because the study of evolutionary integration does not require large samples for any individual species or population (5), an insurmountable barrier to the analysis of variational integration in most rare or extinct taxa, it is a promising approach for analysis of fossil datasets, particularly in combination with studies of variational integration in better sampled taxa.

Analysis of Modularity in the Cranium of *Smilodon fatalis*. To assess modularity in *S. fatalis*, RV coefficient analysis with 10,000 random partitions was used to test three models: (*i*) two-modules (neurocranium and face); (*ii*) six-modules (as observed in most carnivorans) (6, 7); and (*iii*) seven-modules (separate anterior oral and nasal modules, observed previously for *S. fatalis*, detailed in Table S3) (7). Whereas cluster analyses and RV coefficient analysis support a six-module model of cranial modularity for other carnivorans (6, 7), a seven-module model is a better fit for *S. fatalis* (RV = 0.301, *P* = 0.0148) than is the six-module model

(RV = 0.373, *P* = 0.283) or a more simple two-module (neurocranial vs. facial) model (RV = 0.239, *P* = 0.412; results presented for pit 61/67 *S. fatalis* sample, detailed in *Methods*). This shift in *S. fatalis* relative to all other studied felids, and indeed all other studied placental mammals (6, 7), seems to be a clear case of increasing modularity during the evolution of saber-toothed cats. Interestingly, this increase in cranial modularity is not observed in the convergent evolution of saber-toothery in nimravids, the extinct false saber-toothed cats, but additional data are needed to test whether other saber-toothed felids show similar fragmentation of the anterior facial module. Nonetheless, *S. fatalis* provides an unambiguous example of increased modularity of the facial skeleton, relative to extant mammals, demonstrating the importance of examining the variation recorded in fossil taxa. Whether this increased modularity advanced the evolvability of the facial skeleton is unknown, but further analysis of other saber-toothed forms (7) may provide a valuable comparison for establishing the broader relationship between modularity and evolvability.

Additional Details on Methods for Analysis of *S. fatalis* and *Canis dirus*. All data were subjected to Procrustes superimposition before analysis. Procrustes ANOVA (8) was used on three replicates of specimens, demonstrating that measurement error made a negligible contribution to variation (ranging from 1% to 2% of variation among individuals). Allometry made a small but significant contribution to cranial shape across pits (4.1%, *P* < 0.001 for *S. fatalis*; 4.9%, *P* < 0.001 for *C. dirus*), but not within pits, and correcting for allometry did not change results. Covariance matrix repeatability, estimated by randomly resampling each matrix 10,000 times, was high for all samples, ranging from 0.883 to 0.917 for *S. fatalis* and from 0.875 to 0.924 for *C. dirus* (Table S2). Repeatabilities were used to adjust pitwise matrix correlations by dividing matrix correlations by the square root of the product of their respective repeatabilities (9). Mantel's test (10) was used to establish significance (1,000 permutations) of matrix correlations for all comparisons of FA and overall integration. Resampling (10,000 permutations) was used to generate error distributions for each pit sample's measures of variance and integration. Bonferroni-corrected Mann–Whitney tests were used to establish significance of differences in $\log_{10}$ centroid size, variance, and integration between pit samples. All analyses were conducted in Mathematica 9.0 (Wolfram Research Inc.) and MorphoJ 1.0.5 (11).

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Table S1. Pit age ranges, specimen numbers, log$_{10}$ centroid size, variance, fluctuating asymmetry (FA), overall integration (Int), and correlation between FA and overall integration (FA/Int)

Pit	Age, ky	Specimens	Log size	Variance	FA	Int	FA/int
Smilodon fatalis							
77	33–40	19	2.687	0.00278	0.000435	0.578	0.286
91	27–28	21	2.686	0.00271	0.000490	0.515	0.430*
13	17–18	24	2.699	0.00280	0.000573	0.426	0.417*
61/67	13–14	33	2.709	0.00331	0.000526	0.360	0.556*
Canis dirus							
77	33–40	8	2.488	0.00256	0.000476	0.421	0.290
91	27–28	17	2.480	0.00287	0.000362	0.296	0.442
13	17–18	26	2.456	0.00307	0.000504	0.236	0.571*
61/67	13–14	26	2.478	0.00330	0.000365	0.253	0.552*

*Significant matrix correlation as determined by Mantel's test ($P < 0.01$ from 10,000 permutations).

Table S2. Adjusted matrix correlations between pit samples for *S. fatalis* and *C. dirus*

	Pit 77	Pit 91	Pit 13	Pit 61
Smilodon fatalis				
Pit 77	**0.883**	0.477	0.500	0.570
Pit 91	0.721	**0.890**	0.546	0.645
Pit 13	0.691	0.731	**0.900**	0.676
Pit 61	0.714	0.750	0.745	**0.917**
Canis dirus				
Pit 77	**0.875**	0.460	0.530	0.465
Pit 91	0.653	**0.924**	0.688	0.659
Pit 13	0.702	0.811	**0.911**	0.960
Pit 61	0.707	0.764	0.816	**0.910**

Lower triangle elements are correlations of overall phenotypic integration. Upper triangle elements are FA correlations between pits. Diagonal elements (in bold) are matrix repeatabilities from 10,000 permutations. All pairwise correlations are significant (Mantel's test, $P < 0.01$).

Table S3. Landmarks for *S. fatalis* and *C. dirus* and module associations used in analysis of *S. fatalis* (*SI Text*)

Landmark	Module
Anterior midline suture of premaxilla*	N
Nasal–anterior midline suture*	N
Nasal–premaxilla suture anterior–right*	N
Nasal–premaxilla suture anterior–left*	N
Anterior border of canine at alveolus–left*	A
Anterior border of canine at alveolus–right*	A
Canine–mesial extreme–left*	A
Canine–mesial extreme–right*	A
Posterior border of canine at alveolus–left*	A
Posterior border of canine at alveolus–right*	A
Premaxilla–maxilla ventral midline suture*,[†]	A
Anterior border of P3 at alveolus–left*,[†,‡]	M
Anterior border of P3 at alveolus–right*,[†,‡]	M
Anterolateral border of P4 alveolus–left*	M
Anterolateral border of P4 alveolus–right*,[†]	M
Jugal–maxilla ventral suture–left*,[†]	M
Jugal–maxilla ventral suture–right*,[†]	M
Maxilla-palatine midline suture*,[†,‡]	M
Medial border of P4 at widest point of alveolus–left*,[†,‡]	M
Medial border of P4 at widest point of alveolus–right*,[†,‡]	M
Posterior border of palatine at midline*,[†]	M
Postero-lateral border M2–left[†]	—
Medial M2 alveolus–left[†]	—
Medial M2 alveolus–right[†]	—
Medial M1 alveolus–left[†]	—
Medial M1 alveolus–right[†]	—
Posterior of carnassial at alveolus–left*	M
Posterior of carnassial at alveolus–right*	M
Jugal–maxilla–lacrimal suture–right*,[†,‡]	O
Jugal-maxilla-lacrimal suture–left*,[†,‡]	O
Lacrimal–frontal–maxilla suture–left*,[†,‡]	O
Lacrimal–frontal–maxilla suture–right*,[†,‡]	O
Maxilla–frontal–nasal suture–left*,[†,‡]	O
Maxilla–frontal–nasal suture–right*,[†,‡]	O
Nasals–frontal midline suture*,[†]	O
Postorbital process base (jugal)–left*	O
Postorbital process base (jugal)–left*	O
Postorbital process tip (frontal)–left*	O
Postorbital process tip (frontal)–right*	O
Frontal–parietal–alisphenoid suture–left*,[†,‡]	V
Frontal–parietal–alisphenoid suture–right*,[†,‡]	V
Parietal–Frontal midline suture*,[†]	V
Parietal–squamosal–alisphenoid–left*,[†,‡]	V
Parietal–squamosal–alisphenoid–right*,[†,‡]	V
Parietals–occipital midline suture*	V
Posterodorsal tip of occiput at midline*	V
Basioccipital–basisphenoid–bulla suture–left*,[†,‡]	Z
Basioccipital–basisphenoid–bulla suture–right*,[†]	Z
Basisphenoid–basioccipital midline suture*,[†,‡]	Z
Basisphenoid–presphenoid suture–left*,[†,‡]	Z
Basisphenoid–presphenoid suture–right*,[†,‡]	Z
Bulla–anterior medial extreme–left*,[†,‡]	Z
Bulla–anterior medial extreme–right*,[†,‡]	Z
Jugal–squamosal ventral suture–left*	Z
Jugal–squamosal ventral suture–right*	Z
Postglenoid process lateral extreme–left*,[†,‡]	Z
Postglenoid process lateral extreme–right*,[†]	Z
Antero-medial point of mastoid process–left*,[†]	B
Antero-medial point of mastoid process–right*,[†]	B
Basion*,[†,‡]	B
Bulla–posterior lateral extreme–left*,[†]	B
Bulla–posterior lateral extreme–right*,[†]	B

Table S3.   Cont.

Landmark	Module
Mastoid process ventral tip–left*,†	B
Mastoid process ventral tip–right*,†	B
Occipital condyle–extreme–left*,†,‡	B
Occipital condyle–extreme–right*,†,‡	B
Paraoccipital process tip–left*,†	B
Paraoccipital process tip–right*,†	B

Module associations reflect the seven-module model, as follows: A, anterior oral; B, basicranium; M, molar/palate; N, nasal; O, orbit; V, vault; Z, zygomatic/pterygoid [A and N are grouped in most therian mammals (1)]. —, landmarks gathered only for *C. dirus* and thus not included in analyses of modularity for *S. fatalis*.

*Inclusion in the 67 landmark set used in analysis of modularity for *S. fatalis*.
†Inclusion in the 34 landmark dataset for all analyses of *C. dirus*.
‡Inclusion in the 38 landmark subset for all analyses of *S. fatalis* except for analyses of cranial modularity.

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