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Дарья Савельева

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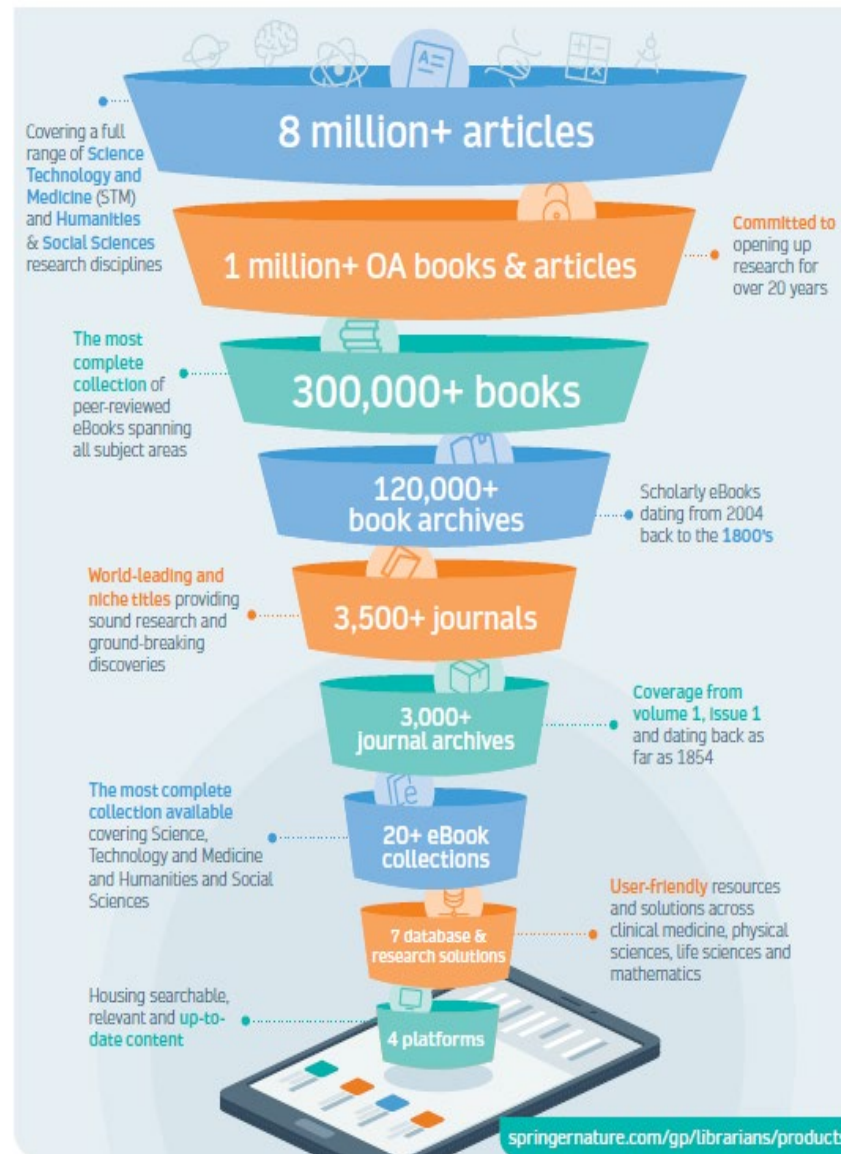
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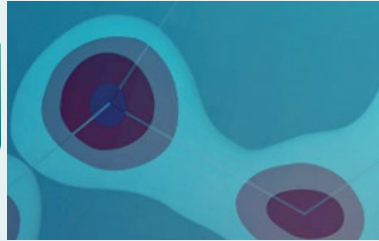
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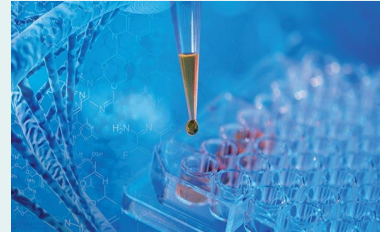
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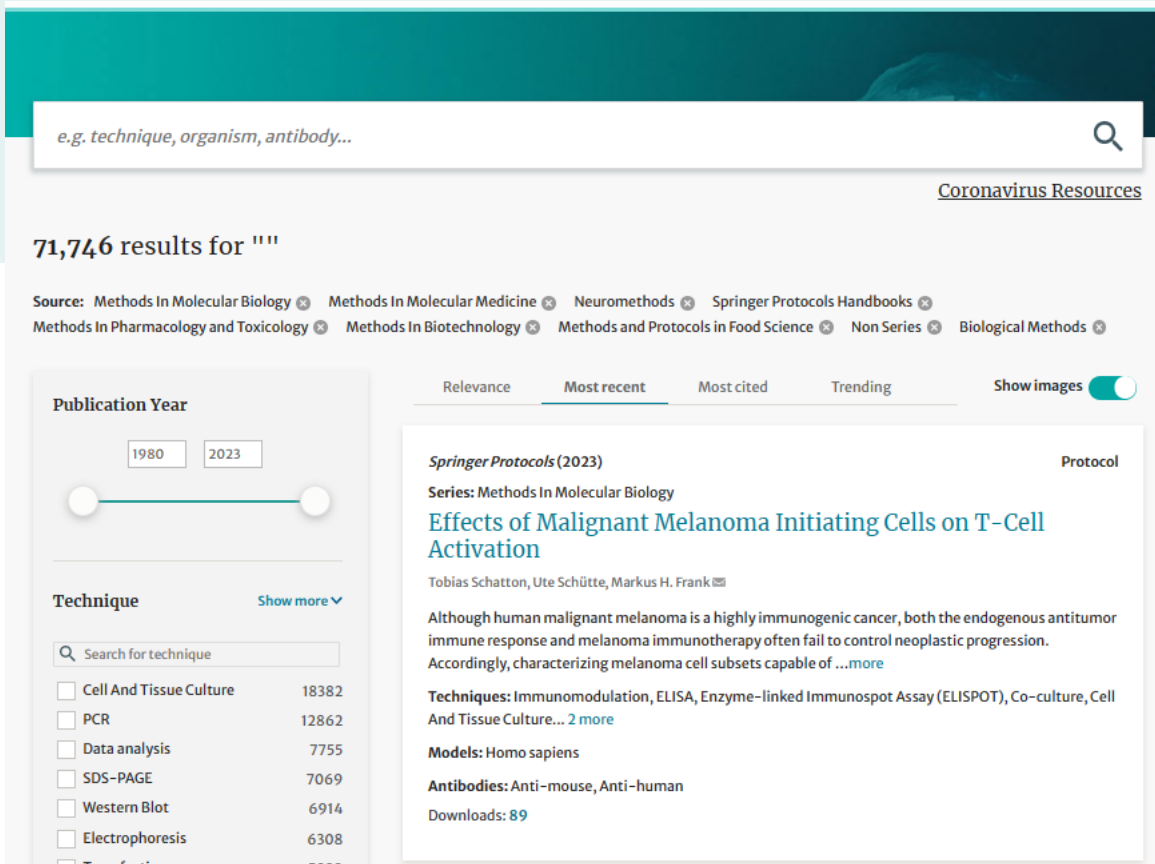
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Effects of Malignant Melanoma Initiating Cells on T-Cell Activation

Tobias Schatton, Ute Schütte, Markus H. Frank

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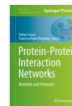
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A Web-Based Protocol for Interprotein Contact Prediction by Deep Learning

Authors [Authors and affiliations](#)

Xiaoyang Jing, Hong Zeng, Sheng Wang, Jinbo Xu

Protocol

First Online: 04 October 2019

460

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Part of the [Methods in Molecular Biology](#) book series (MIMB, volume 2074)

Abstract

Identifying residue–residue contacts in protein–protein interactions or complex is crucial for understanding protein and cell functions. DCA (direct-coupling analysis) methods shed some light on this, but they need many sequence homologs to yield accurate prediction. Inspired by the success of our deep-learning method for intraprotein contact prediction, we have developed RaptorX-ComplexContact, a web server for interprotein residue–residue contact prediction. Given a pair of interacting protein sequences, RaptorX-ComplexContact first searches for their sequence homologs and builds two paired multiple sequence alignments (MSA) based on genomic distance and phylogeny information, respectively. Then, RaptorX-ComplexContact

1 Introduction

Proteins play various roles in cellular and biochemical processes by physically interacting with other proteins or forming protein complexes [1, 2]. Studying protein–protein interactions (PPIs) at residue level is crucial for understanding protein functions in organisms. Experimental techniques have been greatly improved to determine protein complex structure, but they are still low throughput and costly [3, 4]. Therefore, developing effective computational methods to elucidate the 3D structure of a PPI or complex from its sequence is

2 Materials

The following are required and optional materials for the use of RaptorX-ComplexContact server:

1. A personal computer with Internet connection and a web browser with JavaScript enabled. RaptorX-ComplexContact server is compatible with three popular web browsers: Google Chrome, Firefox, and Internet Explorer. Nevertheless, the former two browsers may be slightly better than the third one in visualizing the prediction results.
2. The amino-acid sequences or multiple sequence alignments (MSAs) of the query protein pair in FASTA format. Only the MSAs generated by HHblits are systematically tested although in principle any MSAs shall work.
3. The amino-acid sequences or multiple sequence alignments (MSAs) could also be uploaded to the server as text files.
4. The job name and email address are optional, but a valid email address is strongly recommended since it can facilitate job management and result retrieval.

3 Methods

3.1 Job Submission

1. Open the hyperlink <http://raptorx.uchicago.edu/ComplexContact/> in the web browser.
2. From the menu at the top of the page, select “New job.”

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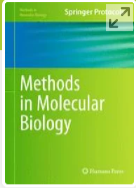
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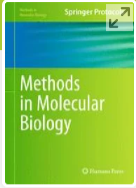
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- **Примечания:** Советы, приемы и рекомендации от автора протокола для исследователей в лабораториях.



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Using DeepLabCut for 3D markerless pose estimation across species and behaviors

Tanmay Nath, Alexander Mathis, An Chi Chen, Amir Patel, Matthias Bethge & Mackenzie Weygandt Mathis

Nature Protocols 14, 2152–2176 (2019) | [Cite this article](#)

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Abstract

Noninvasive behavioral tracking of animals during experiments is critical to many scientific pursuits. Extracting the poses of animals without using markers is often essential to measuring behavioral effects in biomechanics, genetics, ethology, and neuroscience. However, extracting detailed poses without markers in dynamically changing backgrounds has been challenging. We recently introduced an open-source toolbox called DeepLabCut that builds on a state-of-the-art human pose-estimation algorithm to allow a user to train a deep neural network with limited training data to precisely track user-defined

Materials

Equipment

Software

- Operating system: Linux (Ubuntu 16.04 LTS, 18.04 LTS), Windows (10), or MacOS
- Anaconda, a free and open-source distribution of the Python programming language (<https://www.anaconda.com/>). DeepLabCut is written in Python 3.6.x (<https://www.python.org/>) and is not compatible with Python 2
- DeepLabCut: the actively maintained toolbox is freely available at <https://github.com/AlexEMG/DeepLabCut>. The code is written for Python 3.6 (ref. ³⁹) and TensorFlow⁴⁰ for the feature detectors¹⁰
- TensorFlow⁴⁰, an open-source software library for Deep Learning. The toolbox is tested with TensorFlow v.1.0–1.4, 1.8, and 1.10–1.13. Any of these versions can be installed from <https://www.tensorflow.org/install/>
- (Optional) Docker⁴¹; we recommend using the supplied Docker container, which includes DeepLabCut and TensorFlow with GPU support pre-installed. This container builds on the nvidia-docker, which is currently supported only in Ubuntu
- (Optional) Jupyter Notebooks: we provide three Jupyter Notebooks

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DeepLabCut: markerless pose estimation of user-defined body parts with deep learning

Alexander Mathis, Pranav Mamidanna[...] Matthias Bethge

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Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning

P. Gainza, F. Sverrisson, F. Monti, E. Rodolà, D. Boscai, M. M. Bronstein & B. E. Correia

Nature Methods 17, 184–192(2020) | [Cite this article](#)

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Abstract

Predicting interactions between proteins and other biomolecules solely based on structure remains a challenge in biology. A high-level representation of protein structure, the molecular surface, displays patterns of chemical and geometric features that fingerprint a protein's modes of interactions with other biomolecules. We hypothesize that proteins participating in similar interactions may share common fingerprints, independent of their evolutionary history. Fingerprints may be difficult to grasp by visual analysis but could be learned from large-scale datasets. We present MaSIF (molecular surface interaction fingerprinting), a conceptual framework based on a geometric deep learning method to capture fingerprints that are important for specific biomolecular interactions. We showcase MaSIF with three prediction

Methods

Computation of molecular surfaces

All proteins in the datasets were protonated using Reduce⁵⁰, and triangulated using the MSMS program²¹ with a density of 3.0 and a water probe radius of 1.5 Å. Protein meshes were then downsampled and regularized to a resolution of 1.0 Å using pymesh⁵¹. Geometric and chemical features were computed directly on the protein mesh, with the exception of the distance-dependent curvature, which was computed on each patch according to the surface normals of the vertices in the patch.

Decomposition of proteins into overlapping radial patches and computation of features

For each point in the discretized protein surface mesh, a radial patch of geodesic radius of 9 or 12 Å (application-dependent) was extracted to perform an analysis of the surface features of the patch. The choice of radius was empirical, mainly driven by performance and memory constraints. For MaSIF-search we chose 12 Å because we found this to be a good value to cover the buried surface area of many PPIs. This patch size was reused for MaSIF-ligand. A patch of 9 Å was selected for MaSIF-site because the smaller patch allowed us to do multiple convolutional layers within our available memory resources, which we found critical for this application. In the absence of memory constraints, a patch larger than 12 Å would be ideal, as MaSIF's geometric deep learning architecture is capable of assigning different weights to different geodesically clustered kernels.

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Editing the Genome of Human Induced Pluripotent Stem Cells Using CRISPR/Cas9 Ribonucleoprotein Complexes

Michaela Bruntraeger, Meg Byrne, Kathleen Long, Andrew R. Bassett

Genome editing using the CRISPR/Cas9 system has rapidly established itself as an essential tool in the genetic manipulation of many organisms, including human cell lines. Its application to human induced pluripotent stem cells (hiPSCs) allows for the ...[more](#)

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Models: Escherichia coli

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Authors: Zhousi Chen ¹, Xiaoping Duan ¹
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1. Bean, Y., La Bat, P., Ng, H., and Liu, E. (2004). Intron splicing of the yeast genome. *Trends Biochem Sci*, 29, 23–30.
2. Chohan, N., Fornosa, A. E. R., Kalia, G., Girdhac, B. S. A., Paulsen, G. J., Brown, M. K. et al. (2009). Stem cell transcriptome profiling via massive scale mRNA sequencing. *Nature Methods*, 6, 832–839.

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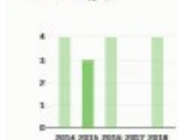
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Models: Escherichia coli
Others: Transcriptome, Ribosomal RNA, Bacteria, 16S, 23S, Next-generation sequencing, Ribosome, Polyketidease

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2019

Three-dimensional virtual refocusing of fluorescence microscopy images using deep learning

nature methods

Authors:

Yichen Wu ^{1,5,6}, Yair Rivenson ^{1,5,6}, Hongda Wang ^{1,5,6}, Yilin Luo ^{1,5,6},
... Aydogan Ozcan ^{1,5,6,7}[show more details](#)

Full text

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Abstract

We demonstrate that a deep neural network can be trained to virtually refocus a two-dimensional fluorescence image onto user-defined three-dimensional (3D) surfaces within the sample. Using this method, termed Deep-Z, we imaged the neuronal activity of a *Caenorhabditis elegans* worm in 3D using a time sequence of fluorescence images acquired at a single focal plane, digitally increasing the depth-of-field by 20-fold without any axial scanning, additional hardware or a trade-off of imaging resolution and speed. Furthermore, we demonstrate that this approach can correct for sample drift, tilt and other aberrations, all digitally performed after the acquisition of a single fluorescence image. This framework also cross-connects different imaging modalities to each other, enabling 3D refocusing of a single wide-field fluorescence image to match confocal microscopy images acquired at different sample planes. Deep-Z has the potential to improve volumetric imaging speed while reducing challenges relating to sample drift, aberration and defocusing that are associated with standard 3D fluorescence microscopy. [less](#)

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Roy Leeuw et al., 2017, Springer Protocols

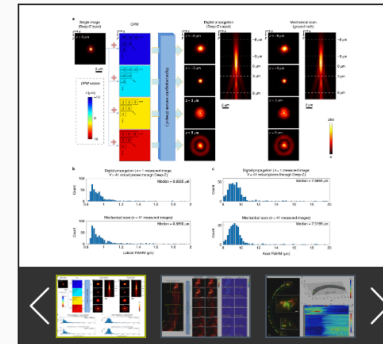
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Vassilis Roukos [✉] et al., 2015, Nature Protocols

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Fig. 1 : Refocusing of fluorescence images using Deep-Z.



Keywords

Techniques:

Confocal Microscopy, Fluorescence Microscopy, Wide-field Microscopy, Deep learning, MetaMorph, [Calcium Imaging](#), ImageJ

Others:

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