

Any 20:

Speaker: Prof. Devi Parikh, Georgia Tech & FAIR

Title: AI for Multimodal Understanding, Creative and Climate Change.

1. AI for Multimodal Understanding, Creativity, Climate Change
2. Time Management

Devi Parikh

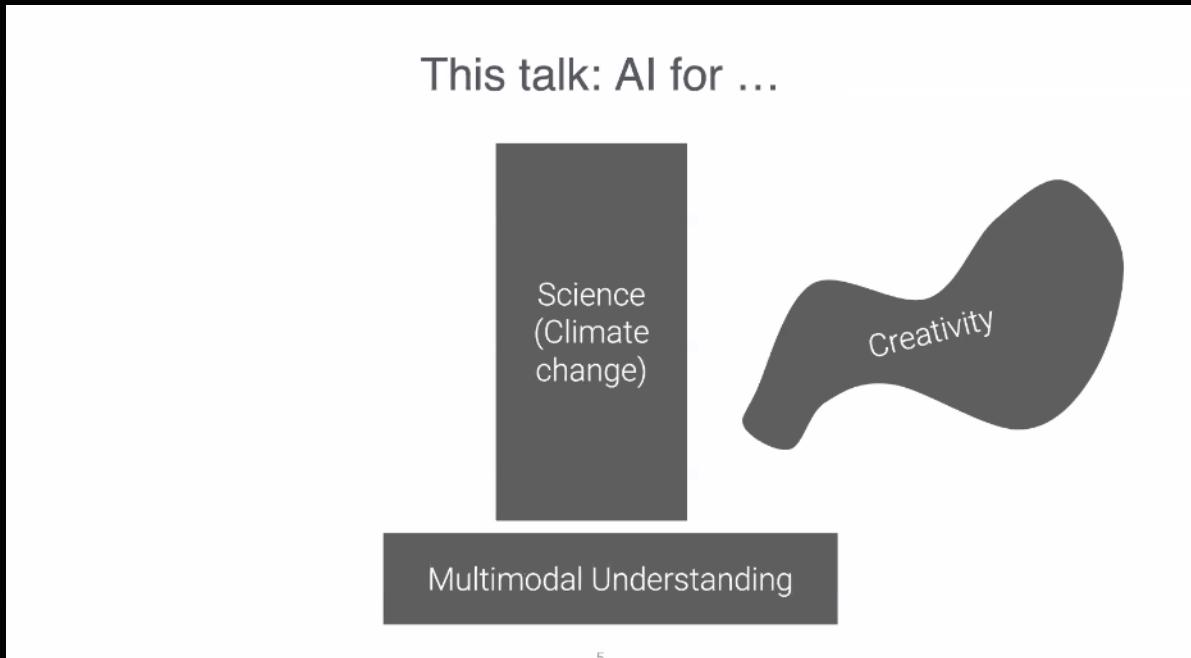


AI for Multimodal Understanding,
Creativity, and Climate Change

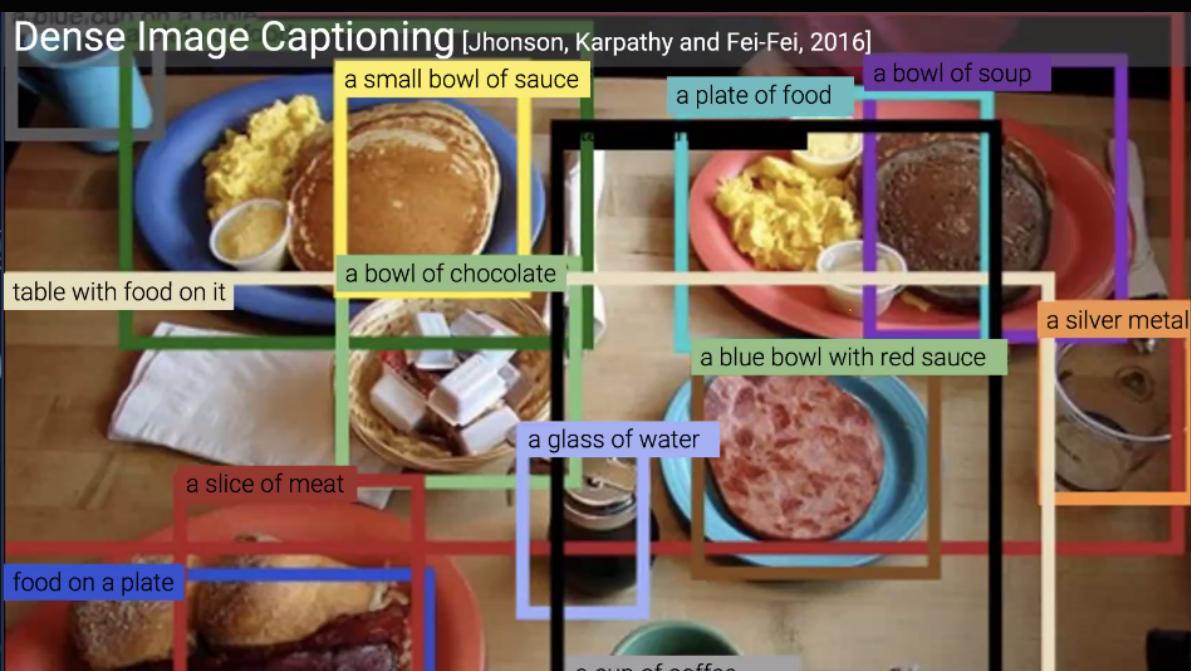
Devi Parikh



This talk: AI for ...



5



Video Description [Rohrbach et al., 2014]



Detailed: A man took a cutting board and knife from the drawer. He took out an orange from the refrigerator. He cut the orange with the knife. He juiced one half of the orange. Then he juiced the other half. The man threw away the skin. He got a glass from the cabinet. Then, he poured the juice into the glass.
Short: A man cut the orange in half. He juiced both halves. Finally, he poured the juice into a glass.

Visual Question Answering [Antol et al., 2015]



What is the kid doing?

Visual Dialog [Das et al., 2017]



A dog with goggles in a motorcycle side car.

Q. Is the motorcycle moving or still?

A. It's parked.

Q. What kind of dog is it?

A. Looks like a beautiful pit bull mix.

Q. What color is it?

A. Light tan with a white patch that runs up to bottom of his chin.

Applications



Aid visually impaired individuals



Navigate unstructured visual data



Leverage multi-modal info



Detect hateful content



Augmented/virtual reality assistance

13

Image Captioning



Man in blue wetsuit is surfing on wave

Karpathy and Fei-Fei (Stanford) 2015

14

Image Captioning



A car is parked in the middle of nowhere

Kiros et al. (University of Toronto) 2015

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Visual Question Answering: Pythia

[Winning entry in 2018 challenge]



Q: What is the cat wearing?
A: Hat



Q: What is the weather like?
A: Rainy



Q: What surface is this?
A: Clay



Tina Jiang Vivek Natarajan Xinlei Chen

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Visual Question Answering: Pythia

[Winning entry in 2018 challenge]



Q: What is the weather like?
A: Sunny



Q: What color is the cat's eyes?
A: Green



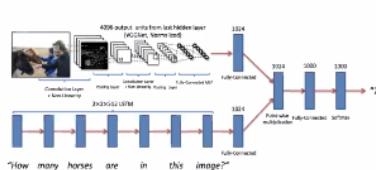
Q: What toppings are on the pizza?
A: Mushrooms



Tina Jiang Vivek Natarajan Xinlei Chen

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Task- and dataset-specific models



Visual Question Answering [Antol et. al. 2015]

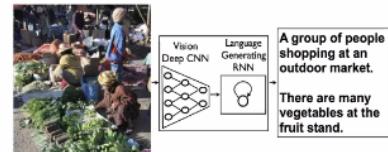
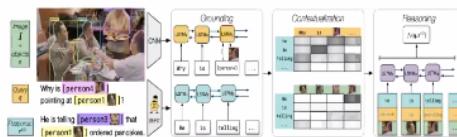
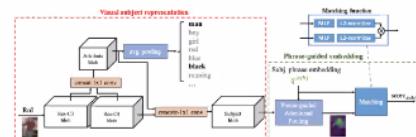


Image Captioning [Vinyals et. al. 2015]



Visual Commonsense Reasoning [Zellers et. al. 2018]



Refer Expression [Yu et. al 2018]

Task- and dataset-specific models



VQA model:

Q: What is the man making?

A: Cake

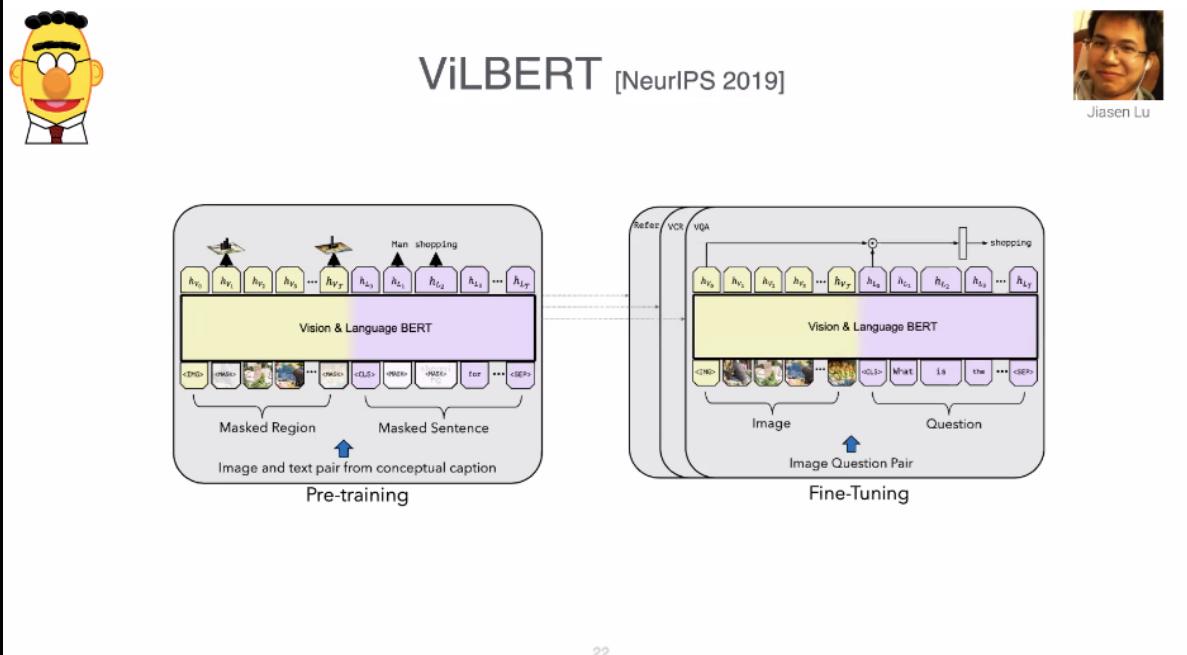
Captioning model:

An older man is wearing an apron and making pizza

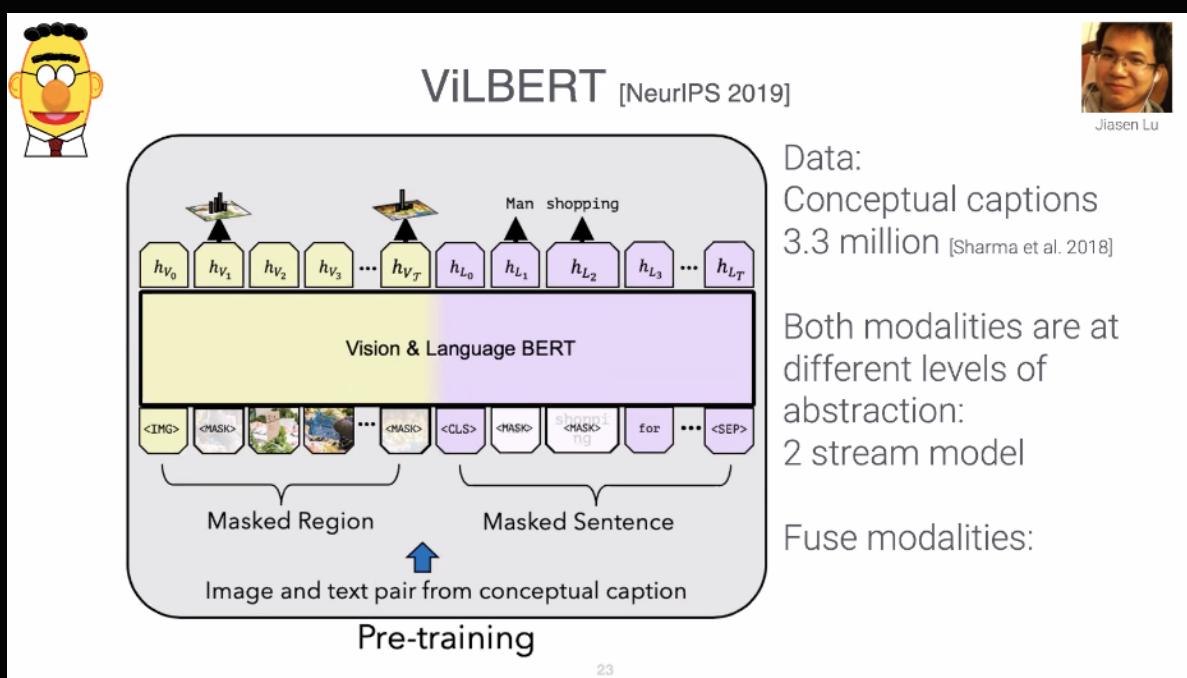
Common model for visual grounding

Leverage for a variety of vision-and-language tasks

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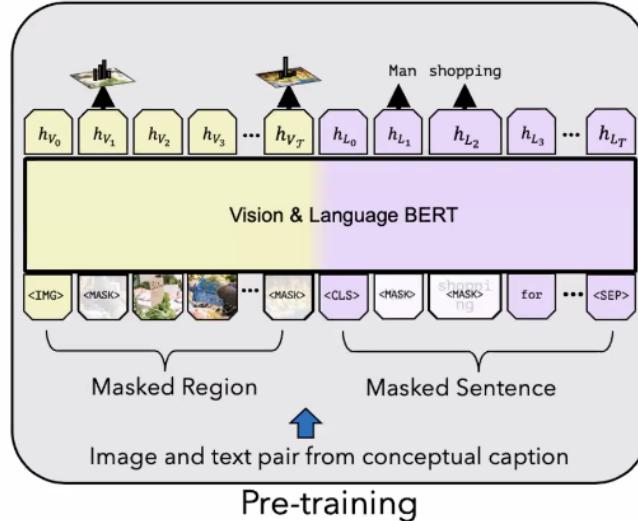


ViLBERT [NeurIPS 2019]



5 downstream tasks

ViLBERT outperformed SOTA on all



24



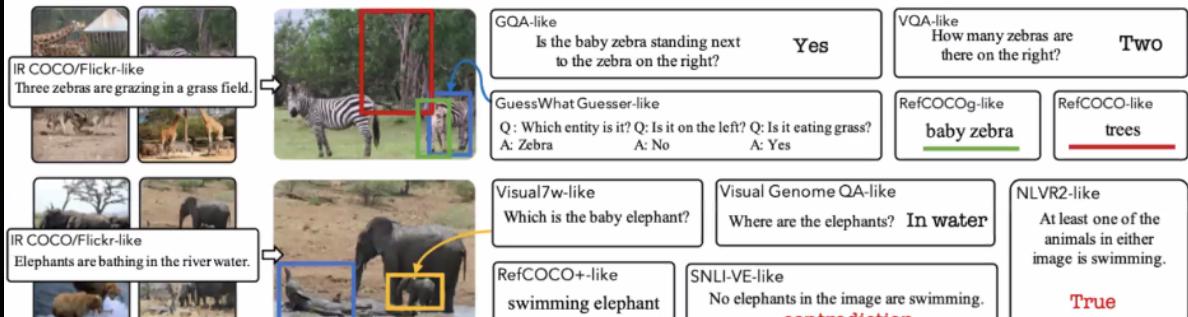
ViLBERT Multi-Task [CVPR 2020]



1 model for 12 tasks!

Higher performance, 1/12th the model size!

SOTA on 7 after fine-tuning



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ViLBERT Multi-Task [vilbert.cloudcv.org]



CloudCV: ViLBERT Multi-Task Demo

A simple ViLBERT Multi-Task model can perform 8 of the 12 vision and language tasks learned from 12 datasets! Datasets: VQA v2, GQA, Visual Genome QA, RefCOCO, RefCOCO+, RefCOCOg, Visual7W, GuessWhat, COCO Retrieval, Flickr8k Retrieval, SNLI-VE, NLVR2.

More details about the ViLBERT Multi-Task paper can be found [here](#).

Browsers currently supported by the demo: Google Chrome, Mozilla Firefox

- How it works
1. You upload an image.
 2. Our servers run the deep-learning based algorithm.
 3. Results and updates are shown in real-time.

Result

Visual Task:
Visual question answering (e.g., VQA)
Visual reasoning (e.g., RefCOCO)
Visual captioning (e.g., Flickr8k)
Answering questions (e.g., NLVR2)
Answering multiple-choice questions (e.g., SNLI-VE)
Visual reasoning (e.g., COCO-QA)
Image caption generation (e.g., RefCOCO)
Image retrieval (e.g., Flickr8k)

Credits

Built by [@rishabh Jain](#)

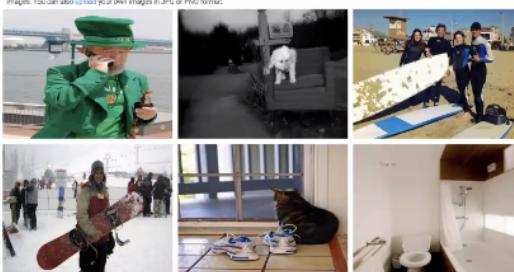
Acknowledgement:

We thank [@jiasen Lu](#) for his help.

Try ViLBERT Multi-Task on sample images

Select one or more images to send to our servers. Most tasks rely on one image. If you're interested in matching a caption to a pair of images (e.g., NLVR2), select 2 images. For image retrieval, select 2 to 4 images. You can also [upload your own images](#) in JPG or PNG format.

Show me images



Matching is pre-computed for these images. They are treated as a fresh batch at every click.

OR

Upload your own images

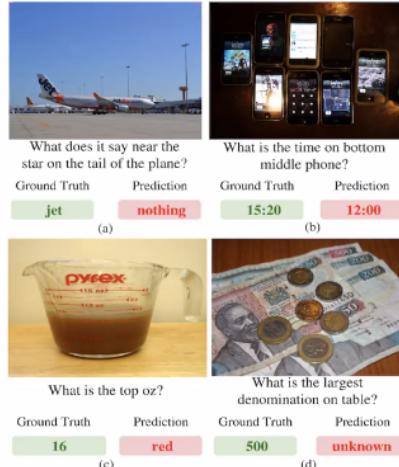
http://.../file was selected

Open Next

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Challenges

Reading and reasoning about text in images
[CVPR 2019]

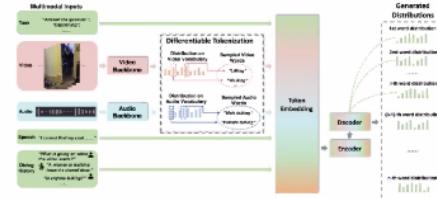


Incorporating external knowledge
[CVPR 2021]



Which liquid here comes from a citrus fruit?

Video [CVPR 2021]



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MMF (A Multimodal Framework): mmf.sh



Amanpreet Singh
Vandanji Goswami

MMF is a modular framework for vision & language multimodal research from Facebook AI Research. MMF contains reference implementations of state-of-the-art vision and language models and has powered multiple research projects at Facebook AI Research. See full list of projects trained or built on MMF [here](#).

MMF is powered by PyTorch, allows distributed training and is an open-source, scalable and fast. Use MMF to bootstrap for your next vision and language multimodal research project by following the [installation instructions](#). Take a look at list of MMF features [here](#).

MMF also acts as a starting codebase for challenges around vision and language datasets (The I2Text Metrics, TextCaps and VQA challenges). MMF was formerly known as Pythia. The next video shows an overview of how datasets and models work inside MMF. Check out MMF's [video overview](#).

Installation

Follow installation instructions in the [documentation](#).

Documentation

Learn more about MMF [here](#).

Citation

If you use MMF in your work or use any models published in MMF, please cite:

```
@inproceedings{2020mmf,
    author = {Amanpreet Singh and Gaurav Balaji and Mohammadreza Vaezi and Jiang, Yu and Chen, Rishabh and Narayan and Akella, Dhruv and Prakash, Deeksha},
    title = {MMF: A Multimodal Framework for vision and language research},
    month = {July},
    year = {2020}
}
```

License

MMF is licensed under BSD license available in [LICENSE](#) file



A modular framework for vision & language multimodal research from Facebook AI Research.

[Get Started](#)



MMF is designed from ground up to let you focus on what matters -- your model -- by providing sensible defaults and letting you quickly comment, iterate and share a state-of-the-art pre-trained backbone out of the box.

Less Boilerplate

MMF is built on top of PyTorch that brings a lot of power to your hands. While it isn't strongly opinionated, it does come with a set of best practices to make things easier.

Powered by PyTorch

MMF is designed to be easy to extend and composable. Through our modular design, you can easily add new components or replace existing ones that don't work for you.

Modular and Composable

MMF is designed to be easy to extend and composable. Through our modular design, you can easily add new components or replace existing ones that don't work for you.

Check out our configuration system's [short guide](#) to easily start up your project.

Installation

Follow installation instructions in the [documentation](#).

Creating a new service endpoint [Optional]

Provide a URL for your endpoint.

Install from source [Recommended]

Provide a URL for your source code.

Install from pip

Provide a URL for your pip package.

Log in

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Why AI for creativity?

AI assisting in creativity
AI challenge
Human-AI collaboration

Creativity is at the core of all progress

Expressing ourselves creatively is a deeply human experience

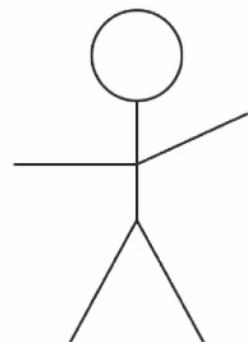
Powerful use of technology

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Music → “Dance” [ICCC 2020]



Purva Tendulkar



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Thematic Typography [ICCC 2019]



Purva Tendulkar



Word book
Theme library



Word car
Theme driving, road, signs



Word witch
Theme Halloween



Word play
Theme Olympics

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Had a wonderful and insightful conversation with my best friend. Many of the things we talked about we were on the same wave-length ... Made a new recipe today and it turned out tasting really well. Will have to remember to put it into my repertoire more often... Had a terrible time getting comfortable when trying to sleep last night. Was so tired today I tried a nap and that didn't go well either.



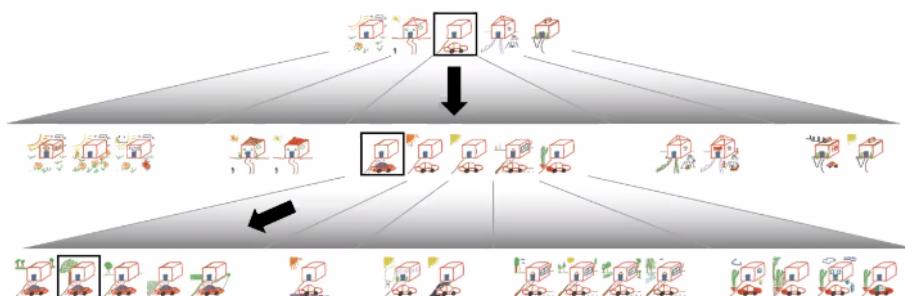
35

Co-creation of Sketches [ICCC 2020]



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Co-creation of Sketches [ICCC 2020]



37

Co-creation of Sketches [ICCC 2020]



Songwei Ge

Creative Sketch Generation

@michalevy

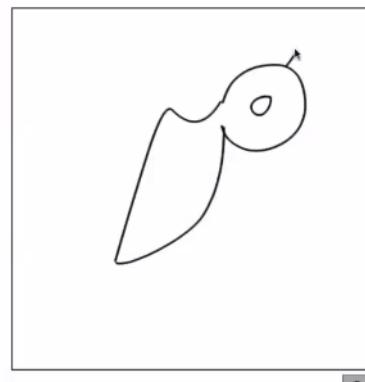
[Slides by Songwei Ge]

51

Creative Sketches

Draw Horn(s)

5 | Next prompt



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Creative Sketch Datasets

Creative Birds (10k)



Creative Creatures (10k)

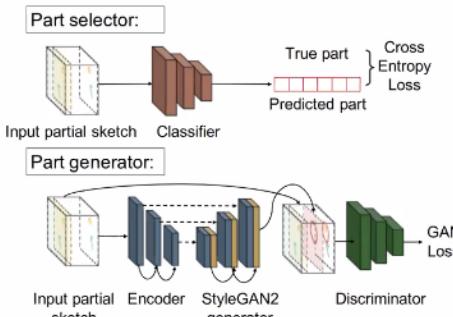


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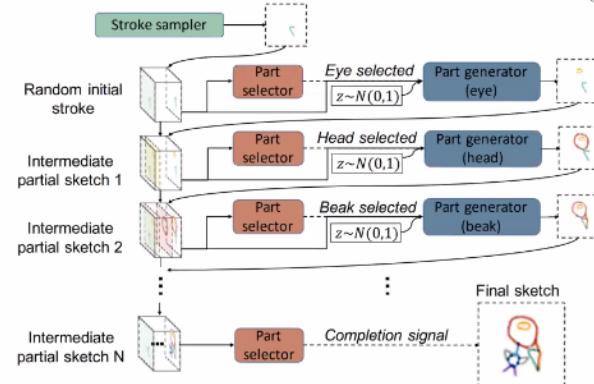


Songwei Ge

DoodlerGAN: Part-based GAN



Training Phase



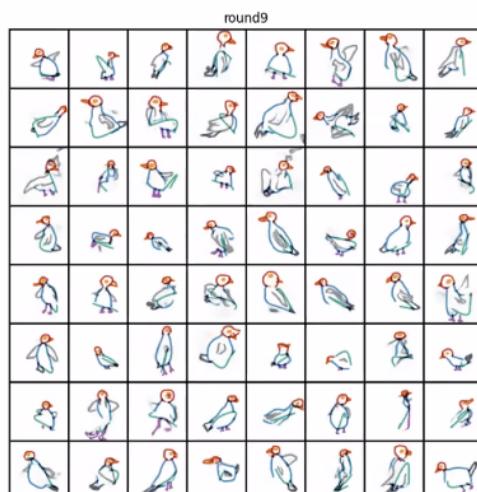
Inference Phase

56



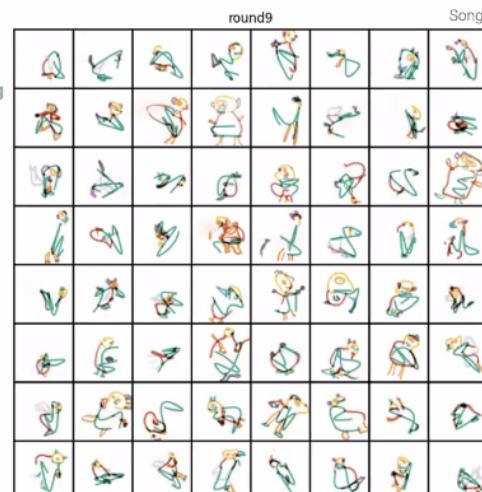
DoodlerGAN Generations

initial
eye
nothing
beak
body
head
legs
mouth
tail
wings



Creative Bird Generation

initial
eye
nothing
arms
beak
body
ears
feet
fin
hair
hands
head
horns
legs
mouth
nose
paws
tail
wings



Creative Creature Generation

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DoodlerGAN Generations → SVG



Hybrids



Our datasets, code, a web demo, and human evaluation protocol will be made publicly available.

Demo

CloudCV: DoodlerGAN - Bird Demo

We will collaboratively draw a sketch of a bird that incorporates a random initial stroke



Click here to draw creative creatures. Check out our [paper](#) on Creative Sketch Generation along with the [code](#) for model training and inference.

Summary

Tremendous scope for progress, exciting future!
What is creativity? How do we operationalize it?
What are the right domains? Tasks? Target users?
How do we evaluate? Benchmarks?
Human-AI collaboration

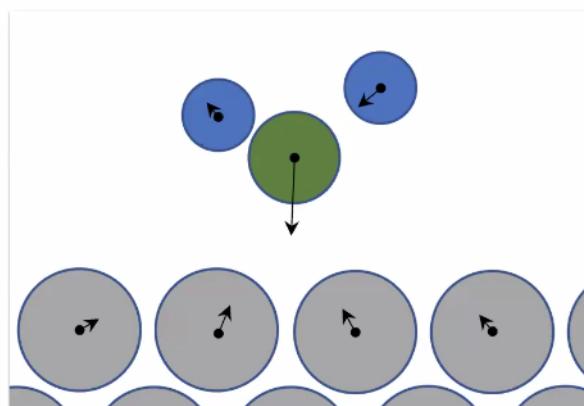
64

AI for Climate Change
(Discovering new catalysts to address energy challenges)

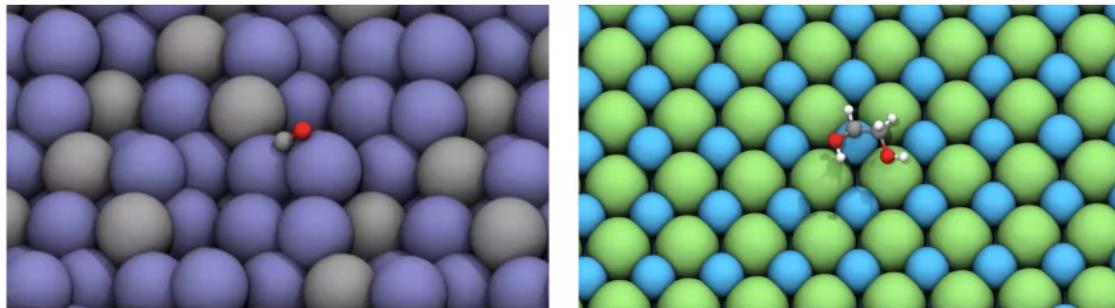
65

Density Functional Theory (DFT)

Computes system energy and per-atom forces



1. Place molecule near the catalyst
2. Find atom positions with lowest energy (relaxation)
 - a. Compute forces
 - b. Update atom positions
 - c. Repeat
3. Use relaxed energy to determine reaction rate



A single relaxation using DFT takes ~8 hours :(



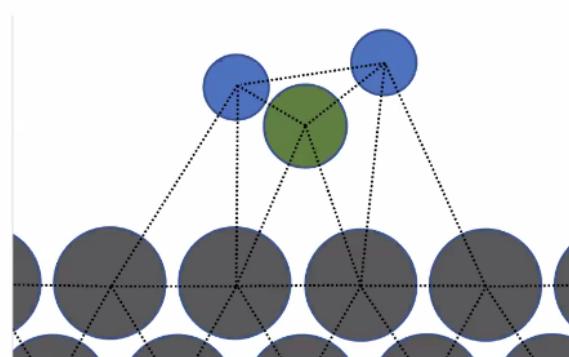
Graph Neural Networks

Node = Atom

Edge = Neighbor

Input:
3D atom positions and
atomic number

Output:
3D atom forces



Open Catalyst Project Dataset (OC20)

1.3M relaxations for training and evaluation

130M+ training examples

70M+ hours to compute on large Facebook servers*

*Facebook servers run on renewable energy

Open Catalyst 2020 (OC20) Dataset download

This page summarizes the dataset download links for S2EF and IS2RE/IS2RS tasks and various splits. The main project website is <https://opencatalystproject.org/>

The Open Catalyst 2020 (OC20) dataset is licensed under a [Creative Commons Attribution 4.0 License](#). Please cite the following paper in any research manuscript using the OC20 dataset:

The Open Catalyst 2020 (OC20) Dataset and Community Challenges. L. Chauvet, A. Das, S. Goyal, T. Levitt, M. Shuaibi, M. Riviere, K. Tran, J. Heras-Domingo, C. Ho, W. Hu, A. Palizhati, A. Sriram, B. Wood, J. Yoon, D. Parikh, C. L. Zitnick, Z. Ulissi, 2020

Structure to Energy and Forces (S2EF) task

For this task's train and validation sets, we provide compressed trajectory files with the input structures and output energies and forces. We provide precomputed LMDBs for the test sets. To use the train and validation datasets, first download the files and uncompress them. The uncompressed files are used to generate LMDBs, which are then used by the dataloaders to train the ML models. Code for the dataloaders and generating the LMDBs may be found in the GitHub repository.

Four training datasets are provided with different sizes. Each is a subset of the other, i.e., the 2M dataset is contained in the 20M and all datasets.

Four datasets are provided for validation set. Each dataset corresponds to a split used to evaluate different types of extrapolation, in domain (id, same distribution as the training dataset), out of domain adsorbate (out_ids), unseen adsorbate, out of domain catalyst (out_cat, unseen catalyst composition), and out of domain both (out_both, unseen adsorbate and catalyst composition).

For the test sets, we provide precomputed LMDBs for each of the 4 subplits (In Domain, OOD Adsorbate, OOD Catalyst, OOD Both).

Each tarball has a README file containing details about file formats, number of structures / trajectories, etc.

Splits	Size of compressed version (in bytes)	Size of uncompressed version (in bytes)	Downloadable link
Train			
all	225G	1.1T	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_train_all.tar
20M	34G	165G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_train_20M.tar
2M	3.4G	17G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_train_2M.tar
200K	344M	1.7G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_train_200K.tar
Validation			
val_id	1.7G	8.3G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_val_id.tar
val_oos_ads	1.7G	8.2G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_val_oos_ads.tar
val_oos_cat	1.7G	8.4G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_val_oos_cat.tar
val_oos_both	1.8G	9.5G	https://dl.fbaipublicfiles.com/opencatalystproject/datasets/zef_val_oos_both.tar

README.md

Open-Catalyst-Project Models

Implements the following baselines that take arbitrary chemical structures as input to predict material properties:

- SchNet
- DimeNet
- Crystal Graph Convolutional Neural Networks (DGCNN).

Installation

[last updated October 10, 2020]

The easiest way of installing prerequisites is via `conda`. After installing `conda`, run the following commands to create a new environment named `exp-models` and install dependencies:

Pre-install step

Install `conda-merge`:

```
pip install conda-merge
```

If you're using system `apt`, then you may want to add the `--user` flag to avoid using `sudo`. Check that you can invoke `conda-merge` by running `conda-merge -h`.

GPU machines

Instructions are for PyTorch 1.6, CUDA 10.1 specifically.

First, check that CUDA is in your `PATH` and `LD_LIBRARY_PATH`, e.g.

```
ls/etc/cuda | tr '-' '\n' | grep cuda
/public/rapids/cuda/10.1/lib64
ls/etc/LIBRARY_PATH | tr '-' '\n' | grep cuda
/public/rapids/cuda/10.1/lib64
```

The exact paths may differ on your system. Then install the dependencies:

```
conda-merge env.common.yml env.gpu.yml > env.yml
conda env create -f env.yml
```

Activate the `conda` environment with `conda activate exp-models`. Install this package with `pip install -e .`. Finally, install the pre-commit hooks:

```
pre-commit install
```

CPU-only machines

Please skip the following if you completed the with-GPU installation from above.

```
conda-merge env.common.yml env.cpu.yml > env.yml
```

An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage

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Abstract

Scalable and cost-effective solutions to renewable energy storage are essential to addressing the world's rising energy needs while reducing climate change. As we increase our reliance on renewable energy sources such as wind and solar, which produce intermittent power, storage is needed to transfer power from times of peak generation to peak demand. This may require the storage of power for hours, days, or months. One solution that offers the potential of scaling to nation-sized grids is the conversion of renewable energy to other fuels, such as hydrogen or methane. To be widely adopted, this process requires cost-effective solutions to running electrochemical reactions. An open challenge is finding low-cost electrocatalysts to drive these reactions at high rates. Through the use of quantum me-

rcers. Meanwhile, solar and wind are projected by 2050 to expand significantly and account for over 70% of renewable energy generation [2]. With this expansion, a unique and potentially limiting challenge arises. Unlike traditional power sources, such as coal, natural gas, and nuclear, power provided by solar and wind is intermittent.

The wind does not always blow, and the sun sets. During these periods, wind and solar plants do not generate any power. Notably, energy demand typically peaks in the early mornings (8am) and evenings (6-7pm) well outside the peak generating time (noon) for solar power [3], Figure 1. On the other hand, during peak mid-day solar power generation, the power from other more conventional sources must be reduced to balance supply and demand. Adjustments in output from conventional plants may not always be able to match the variability of solar and wind power genera-

Summary

Multimodal AI: Vision and language

AI-assisted human creativity

AI for discovering new catalysts to address energy challenges

