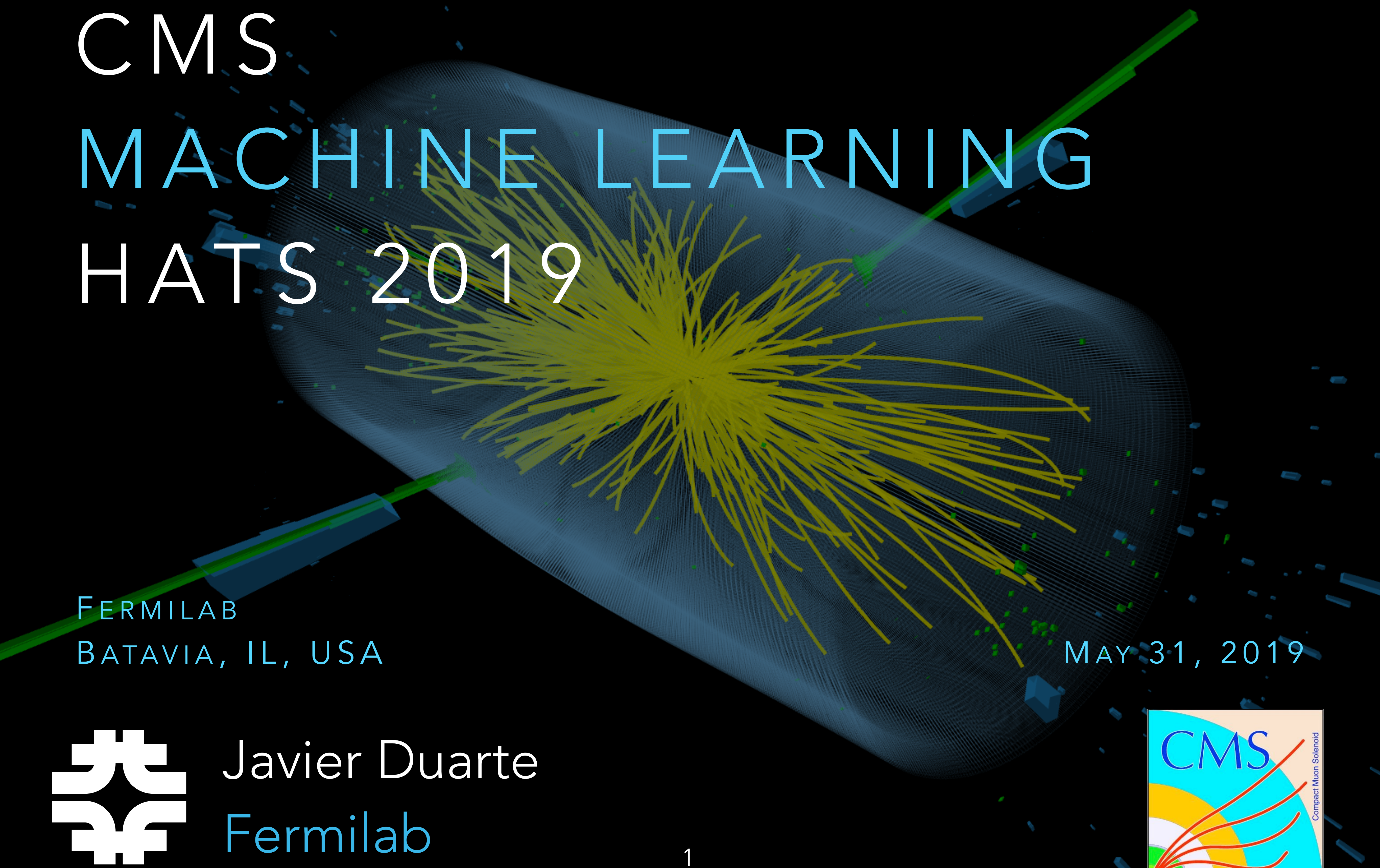
CMS ML HATS 2019

CMS MACHINE LEARNING HATS 2019



Fermilab
Batavia, IL, USA

May 31, 2019

Javier Duarte
Fermilab

OUTLINE

- Overview
- Introduction to artificial neural networks
  - Linear models: perceptron, logistic regression
  - Neural network
  - Backpropagation (chain rule)
  - (Stochastic) gradient descent
  - Practicalities: overfitting, dropout, hyperparameter optimization
- Boosted decision trees
- Tools
  - ML: Keras/TensorFlow, PyTorch
  - CMS/HEP: rootpy, root_numpy, DL4Jets
- Exercises

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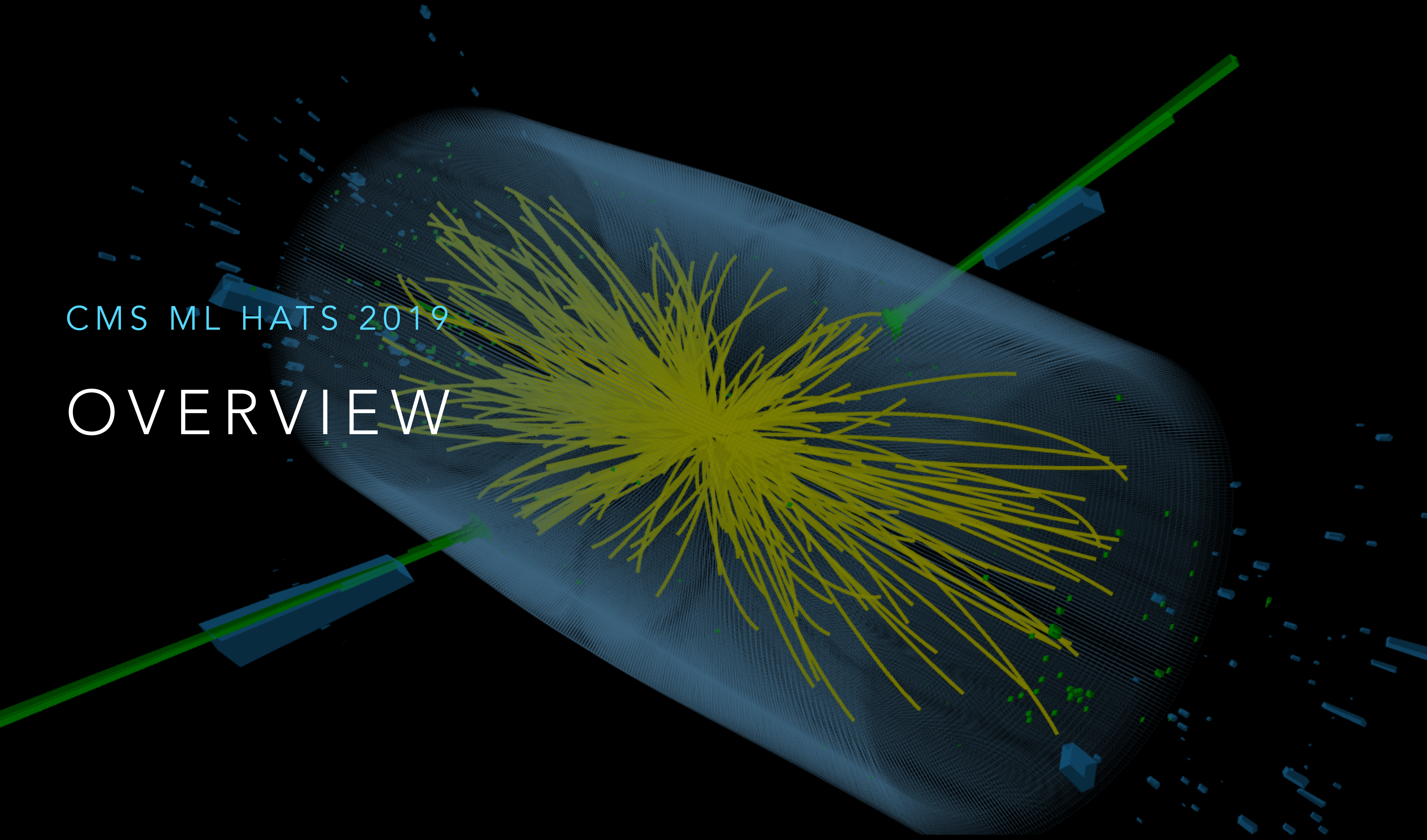
OVERVIEW



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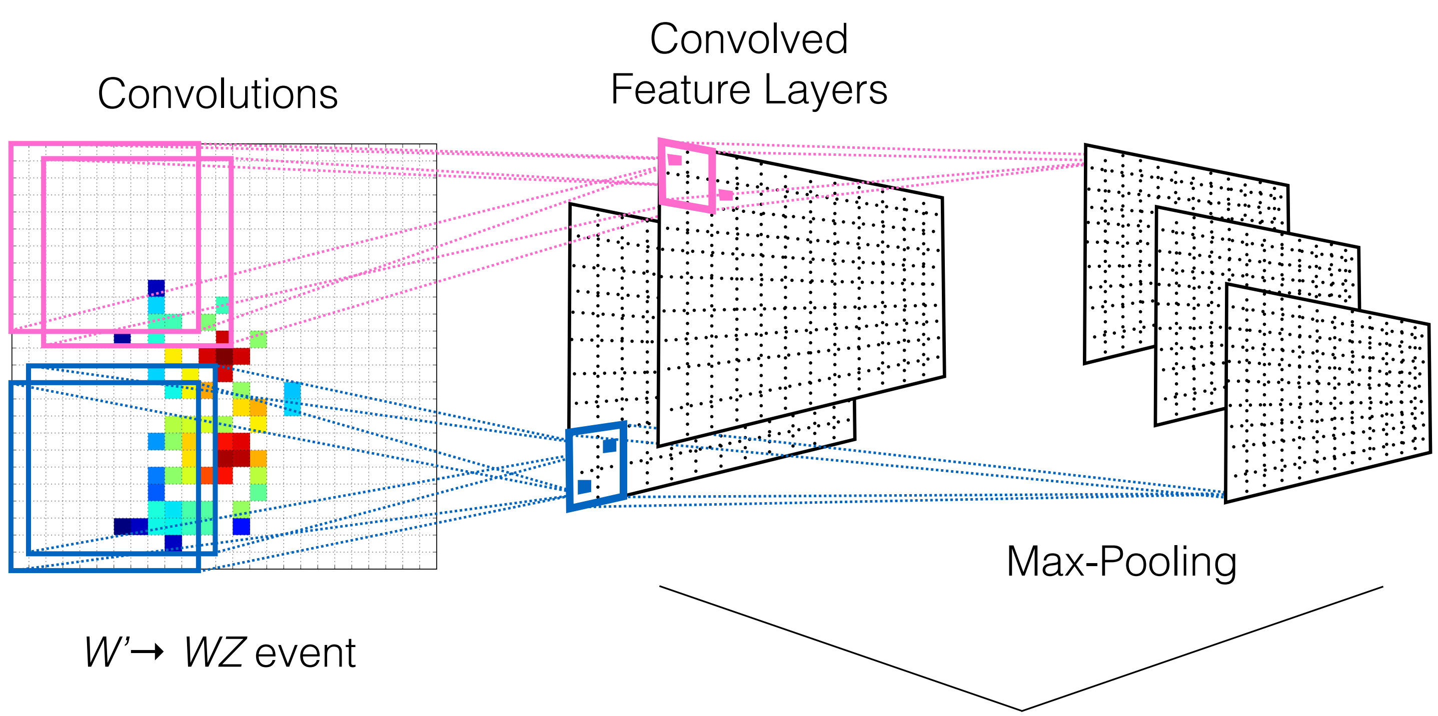
WHAT IS MACHINE LEARNING?

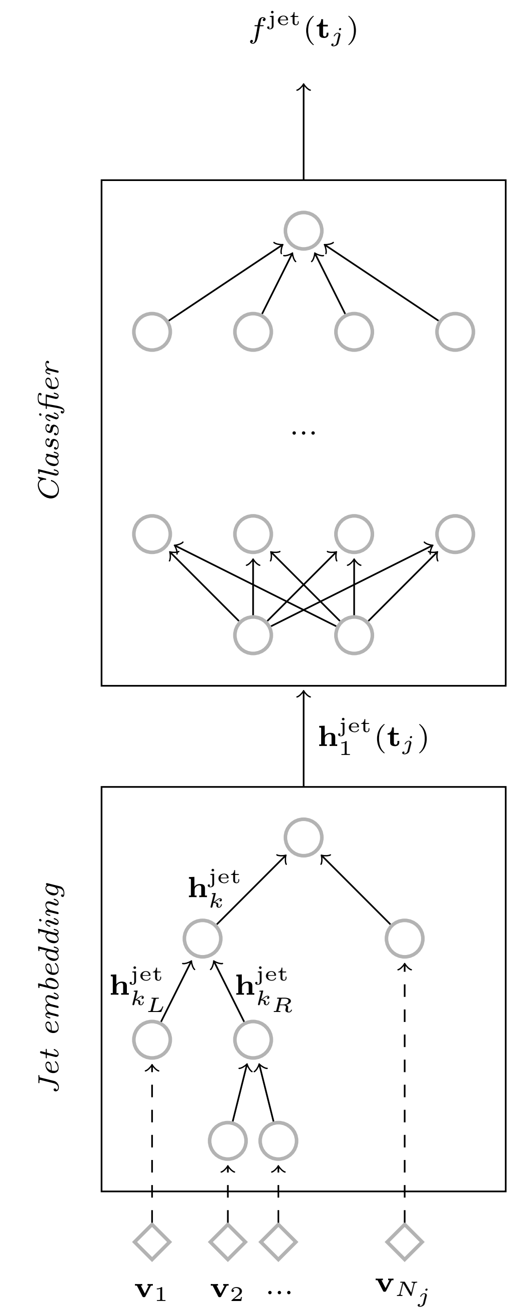
- Learning **mathematical models** from **data** that
  - characterize the **patterns**, regularities, and relationships amongst **variables** in the system
- Three key components:
  - **Model:** chosen mathematical model (depends on the task / available data)
  - **Learning**: estimate statistical model from data
  - **Prediction and Inference**: using statistical model to make predictions on new data points and infer properties of system(s)

MACHINE LEARNING APPS

- Many applications in HEP:
  - Convolutional neural networks using an analogy between calorimeters and images [arXiv:1407.5675, arXiv:1511.05190, arXiv:1704.02124]
  - Recursive neural networks built upon an analogy between QCD and natural languages [arXiv:1702.00748]
  - …



[L. de Oliveira, et al. arXiv:1511.05190]



[G. Louppe, et al. arXiv:1702.00748]

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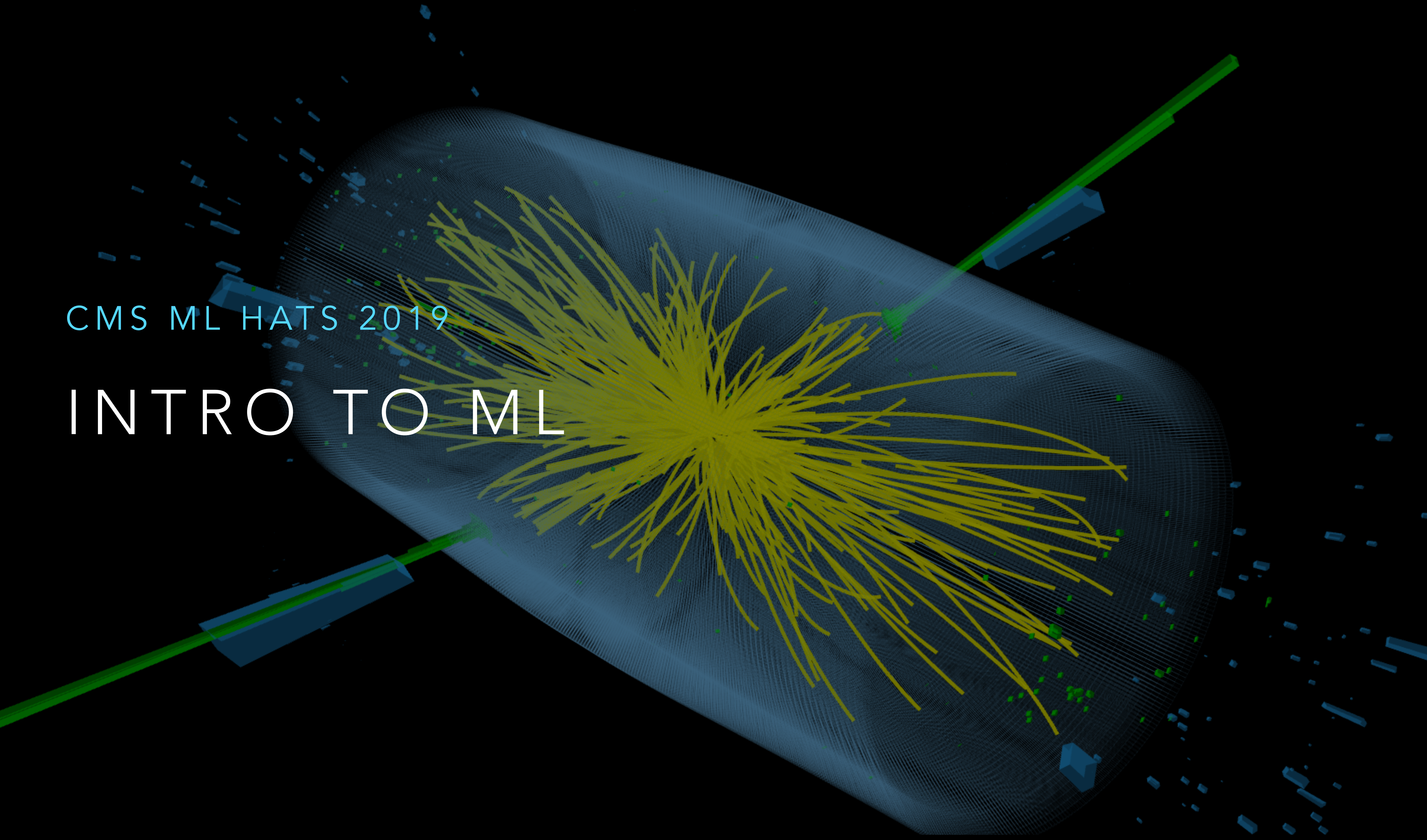
INTRO TO ML



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TYPES OF LEARNING

- Supervised Learning
  - Classification
  - Regression
- Unsupervised Learning
  - Clustering
  - Dimensional reduction
  - Autoencoders
  - …

SUPERVISED LEARNING

- Given N examples with features $\{x_i \in \mathcal{X}\}$ and **targets** $\{y_i \in \mathcal{Y}\}$, learn function mapping **h(x)=y**
  - **Classification**: $\mathcal{Y}$ is a finite set of **labels** (i.e. classes)

$\mathcal{Y} = \{0, 1\}$ for **binary classification**,
encoding classes, e.g. Higgs vs Background

$\mathcal{Y} = \{c_1, c_2, \ldots c_n\}$ for **multi-class classification**

represent with "**one-hot-vector**"

$\rightarrow$ $y_i = (0, 0, \ldots, 1, \ldots 0)$

were k^{th} element is 1 and all others zero for class c_k

SUPERVISED LEARNING

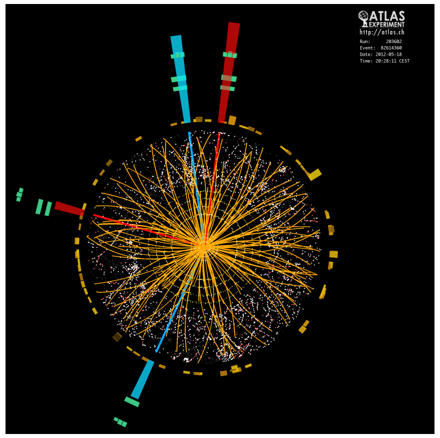
- Given N examples with features $\{\mathbf{x}_i \in \mathcal{X}\}$ and **targets** $\{y_i \in \mathcal{Y}\}$, learn function mapping **$h(x)=y$**
  - **Classification**: $\mathcal{Y}$ is a finite set of **labels** (i.e. classes)
  - **Regression**: $\mathcal{Y}$ = Real Numbers
- Often these are **discriminative models**, in which case we model:

$$h(x) = p(y|x)$$

- Sometimes use **generative models**, estimate joint distribution $p(y, x)$
  - Often estimate class conditional density $p(x|y)$ and prior $p(y)$
  - Use Bayes theorem to then compute:

$$h(\mathbf{x}) = p(y|\mathbf{x}) \propto p(\mathbf{x}|y)p(y)$$

SUPERVISED LEARNING



h(**x**; **w**)
Function with adjustable parameters

Loss Function

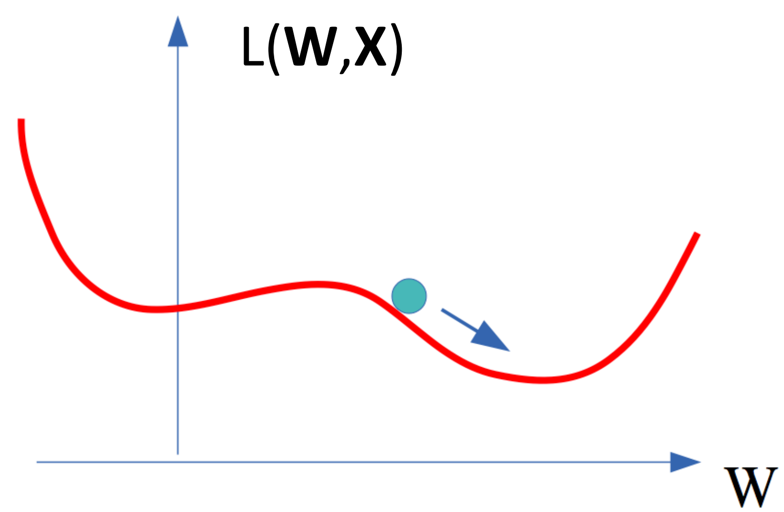
Compare prediction with true label

Loss

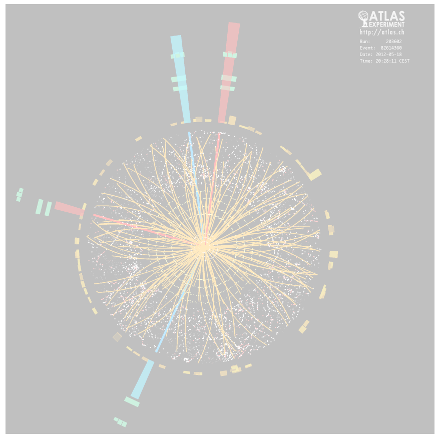
<u>True labels:</u>
Higgs = 1
Bkg = 0

- Design function with adjustable parameters
- Design a Loss function
- Find best parameters which minimize loss
  - Use a labeled *training-set* to compute loss
  - Adjust parameters to reduce loss function
  - Repeat until parameters stabilize
- Estimate final performance on *test-set*

Y. Le Cun



SUPERVISED LEARNING



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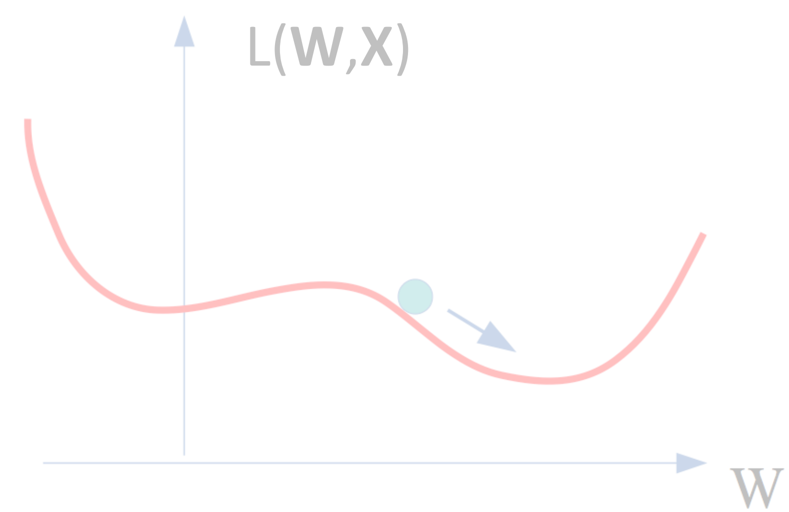
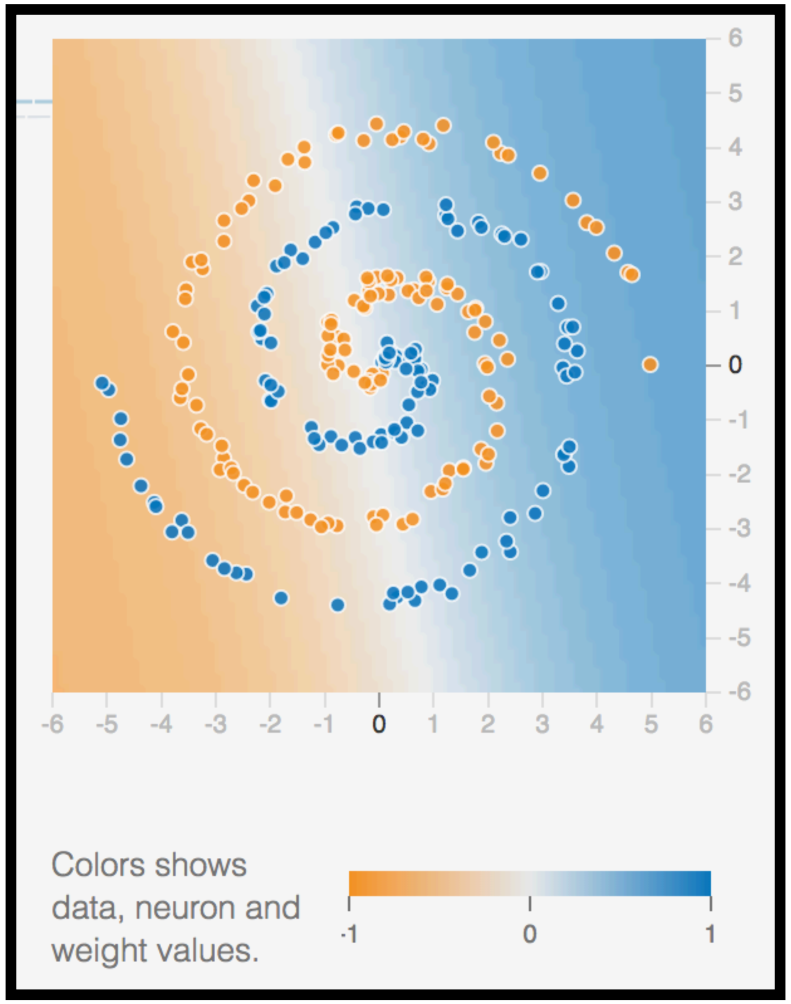
A neural network!

Y. Le Cun



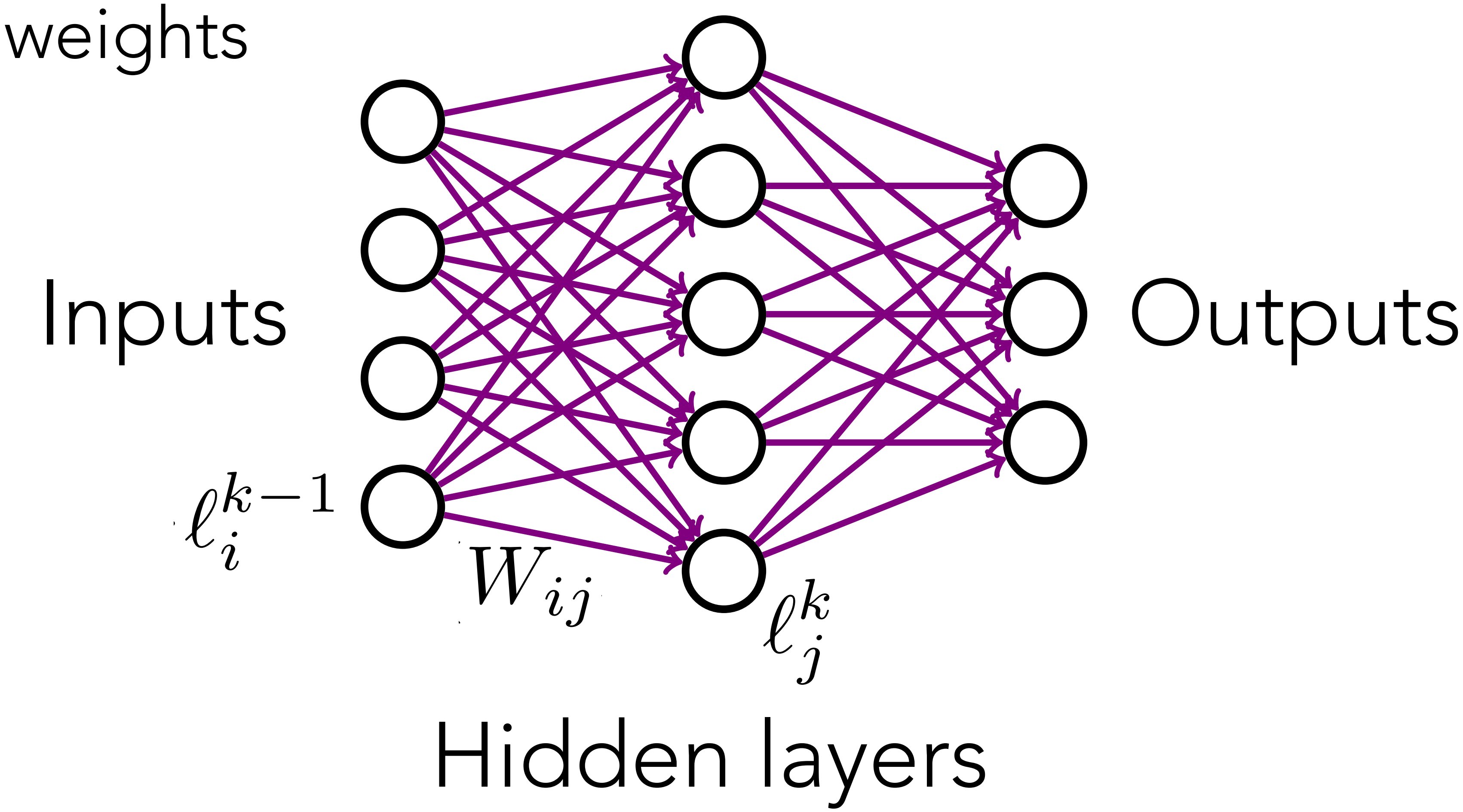
NEURAL NETWORK

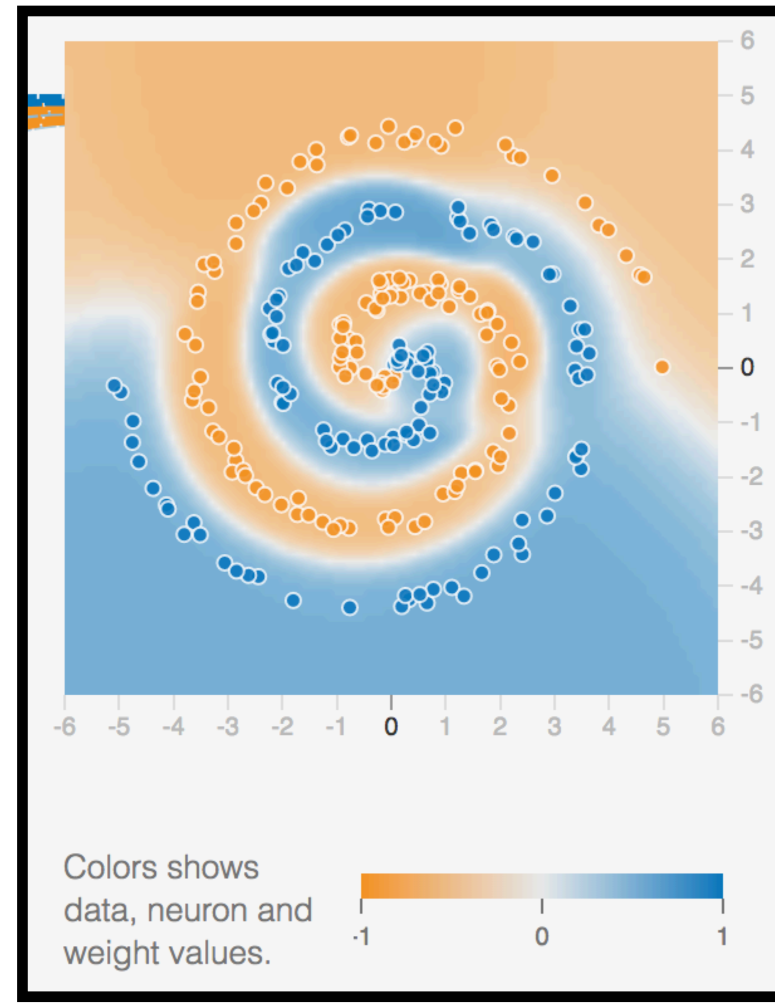
- Universal approximation theorem:
    - Simple neural networks can represent a wide variety of complicated functions.



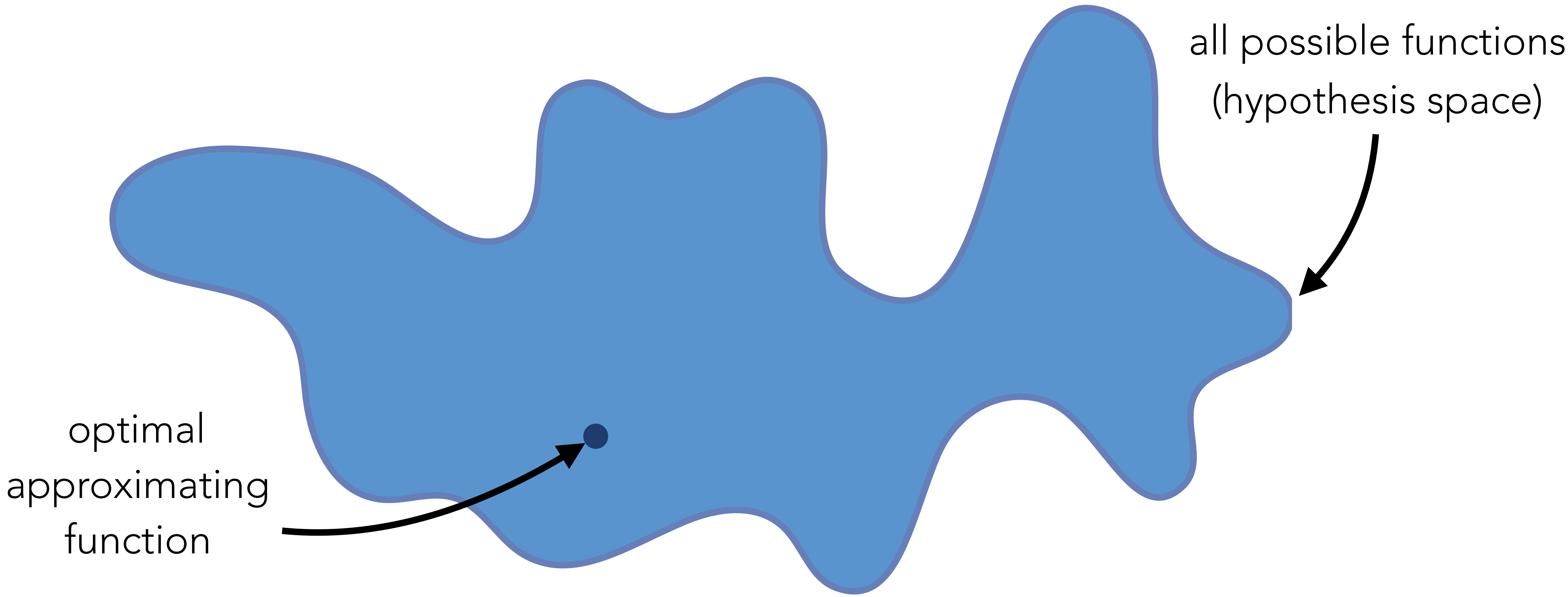
NEURAL NETWORK

- **Multiple layers**: output of previous layer is ***fed forward*** to next layer after applying ***non-linear*** activation function $\boxed{\ell_j^k = \phi(W_{ij}\ell_i^{k-1} + b_j)}$
- **Fully connected**: many independent weights
- **Learning**: Use analytic derivatives and stochastic gradient descent to find optimal weights





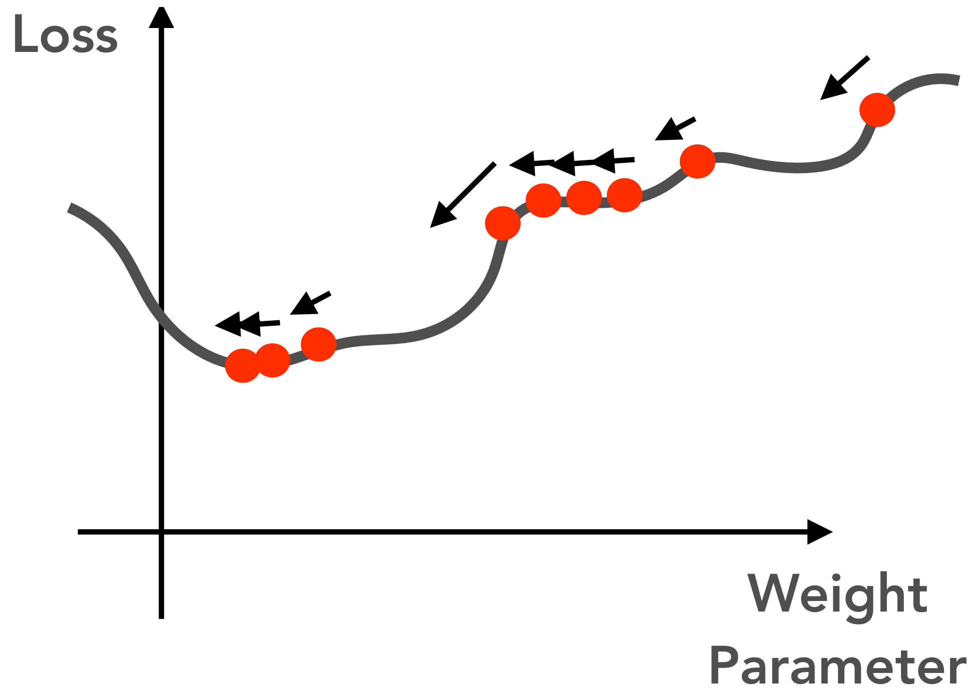
neural networks are universal function approximators,
but we still must find an optimal approximating function



we do so by adjusting the weights

LEARNING = OPTIMIZATION

learning as *optimization*



to learn the weights, we need the **derivative** of the loss w.r.t. the weight

i.e. "*how should the weight be updated to decrease the loss?*"

$$w = w - \alpha \frac{\partial \mathcal{L}}{\partial w}$$

with multiple weights, we need the **gradient** of the loss w.r.t. the weights

$$\mathbf{w} = \mathbf{w} - \alpha \nabla_{\mathbf{w}} \mathcal{L}$$

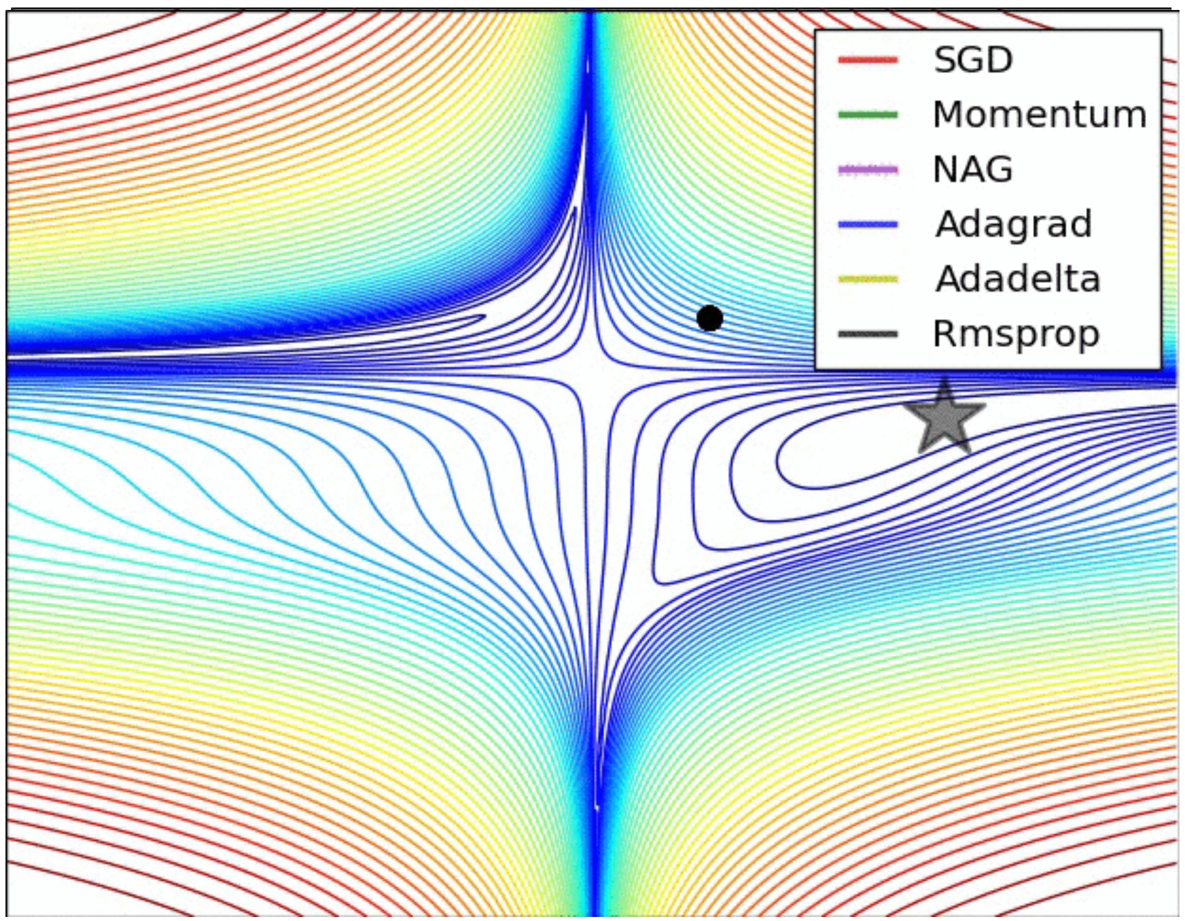
STOCHASTIC GRADIENT DESCENT

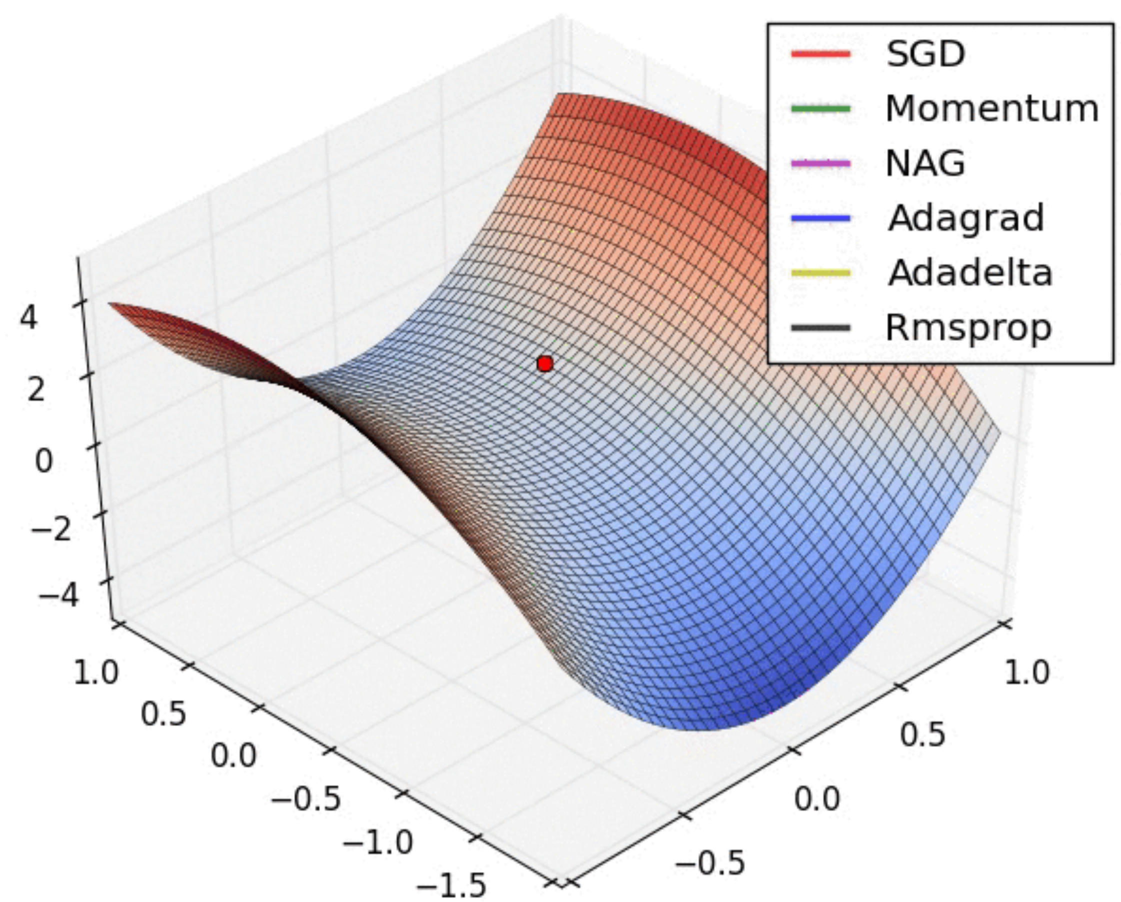
See animated gifs: http://ruder.io/optimizing-gradient-descent/

stochastic gradient descent (SGD): $w = w - \alpha \tilde{\nabla}_w \mathcal{L}$

use *stochastic gradient* estimate to *descend* the surface of the loss function

recent variants use additional terms to maintain "memory" of previous gradient information and scale gradients per parameter





local minima and saddle points are largely not an issue

in many dimensions, can move in exponentially more directions

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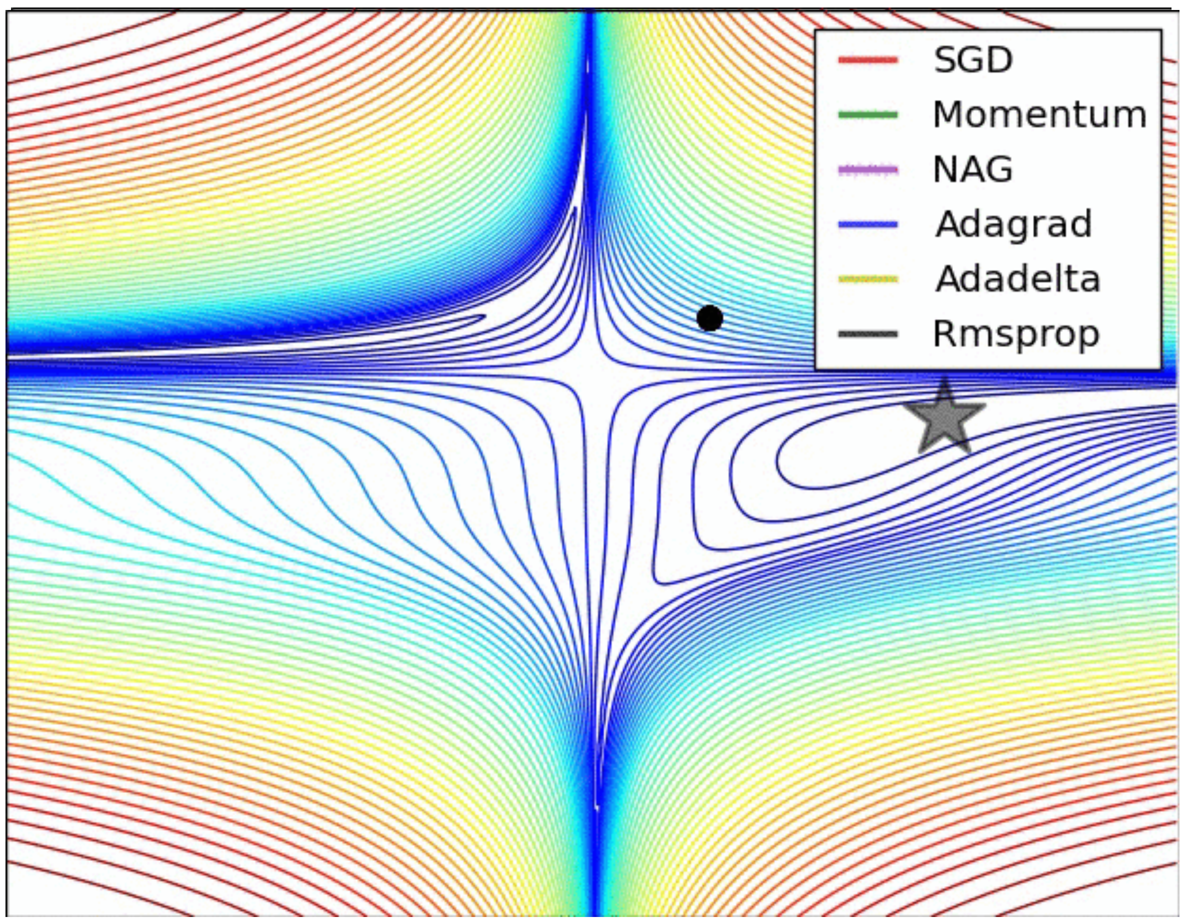

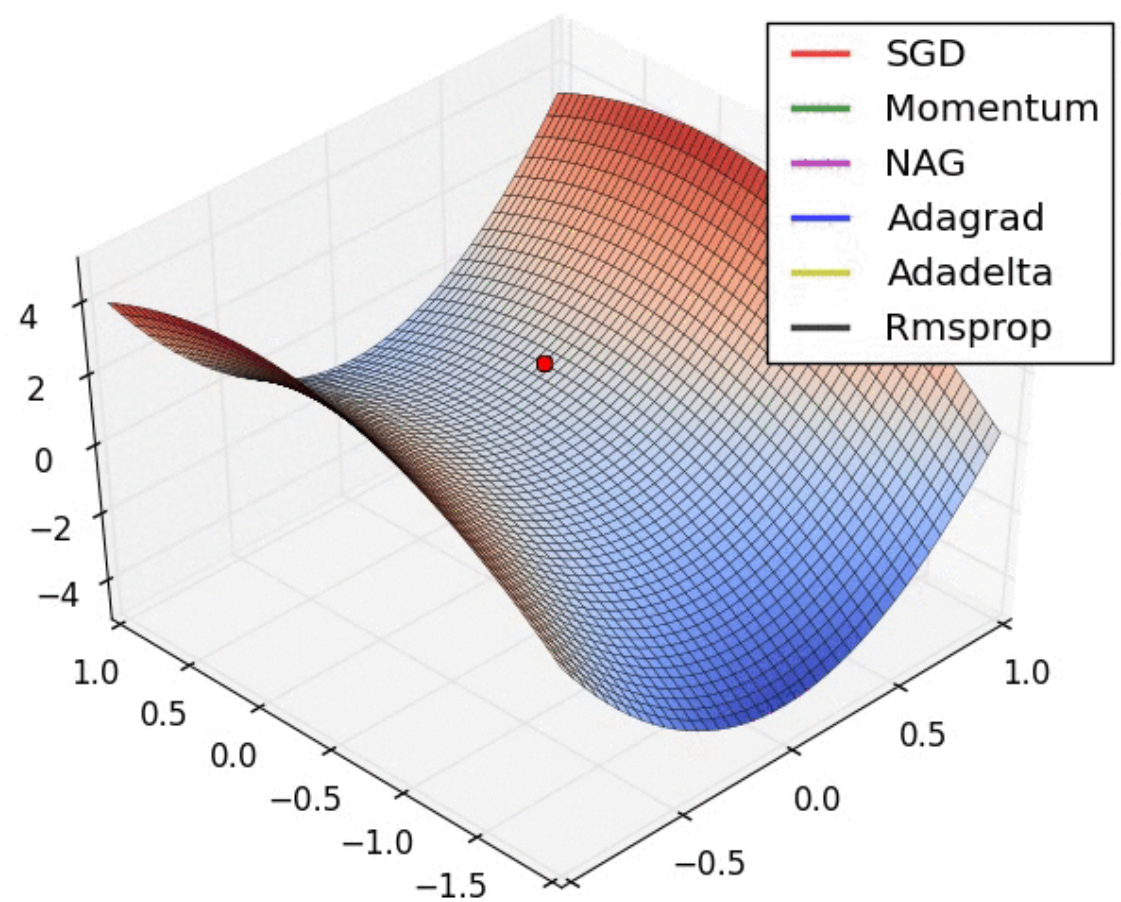

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BACKPROPAGATION

a neural network defines a function of composed operations

$$f_L(\mathbf{w}_L, f_{L-1}(\mathbf{w}_{L-1}, \ldots f_1(\mathbf{w}_1, \mathbf{x}) \ldots))$$

and the loss $\mathcal{L}$ is a function of the network output

⟶ use <u>chain rule</u> to calculate gradients

chain rule example

$$y = w_2 e^{w_1 x}$$

input x output y parameters w_1, w_2

evaluate parameter derivatives: $\frac{\partial y}{\partial w_1}, \frac{\partial y}{\partial w_2}$

define

$v \equiv e^{w_1 x} \longrightarrow y = w_2 v$

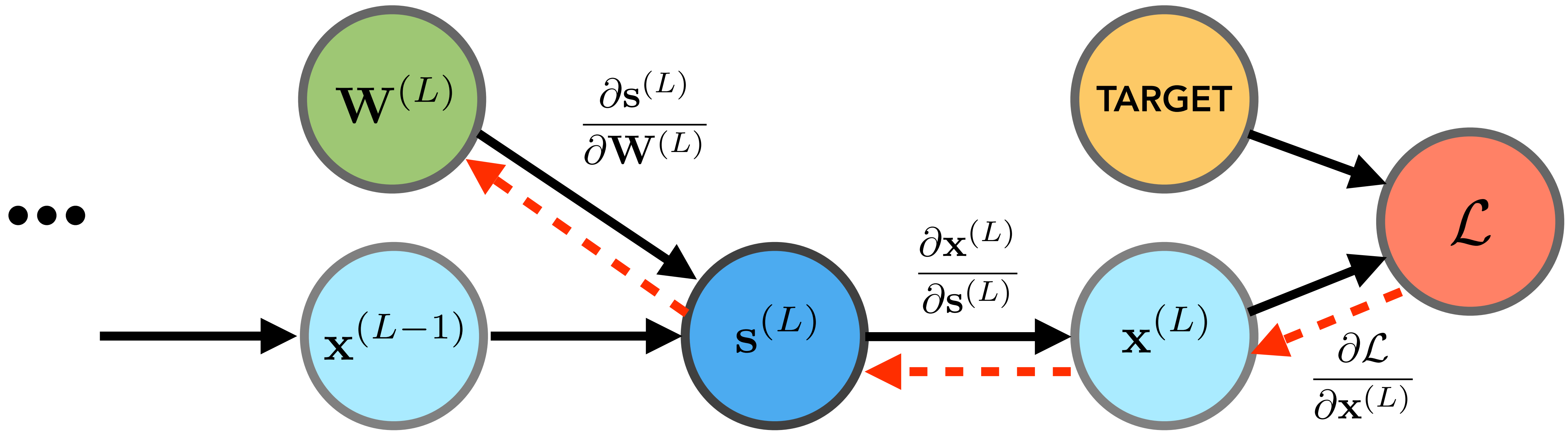
$u \equiv w_1 x \longrightarrow v = e^u$

then $\frac{\partial y}{\partial w_2} = v = e^{w_1 x}$

chain rule

$$\frac{\partial y}{\partial w_1} = \boxed{\frac{\partial y}{\partial v}\frac{\partial v}{\partial u}\frac{\partial u}{\partial w_1}} = w_2 \cdot e^{w_1 x} \cdot x$$

BACKPROPAGATION



$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{W}^{(L)}}$$

depends on the form of the loss

derivative of the non-linearity

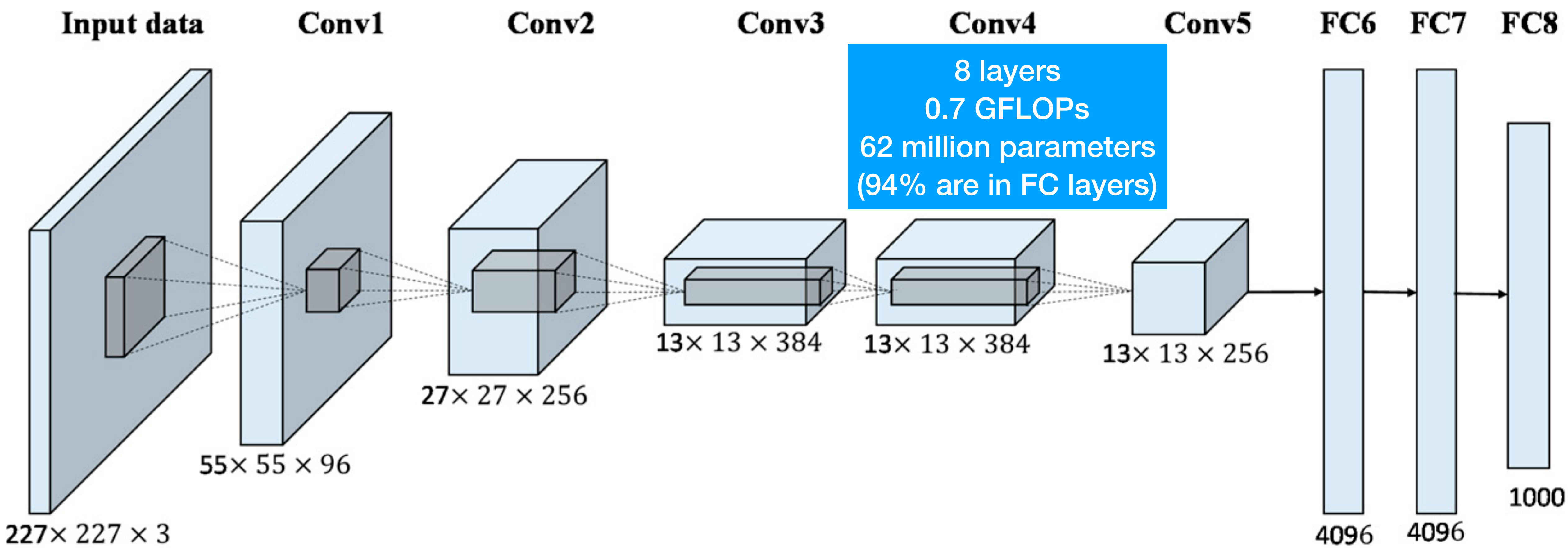
$$\frac{\partial}{\partial \mathbf{W}^{(L)}}(\mathbf{W}^{(L)\intercal}\mathbf{x}^{(L-1)})$$

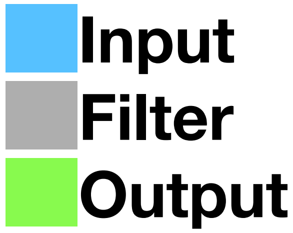
$$= \mathbf{x}^{(L-1)\intercal}$$

CONVOLUTIONAL NETWORKS

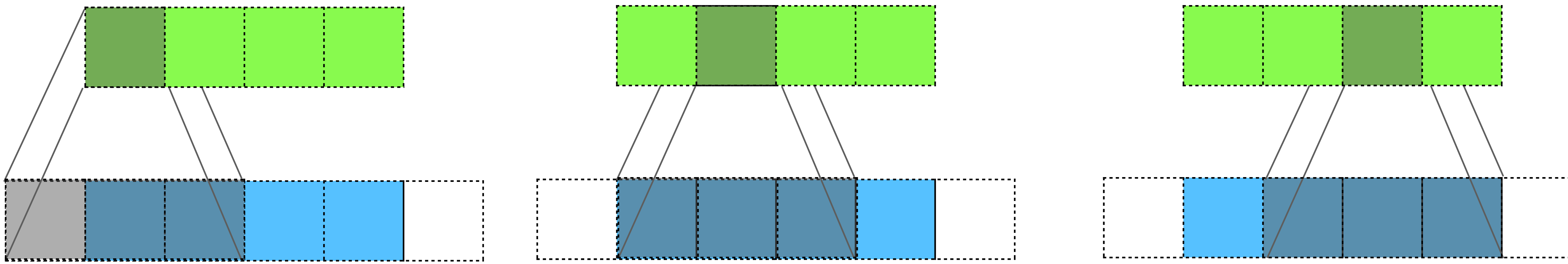
- Main task is computer vision/image recognition
- Control the number of parameters by baking in assumptions like locality and translation invariance to share weights within a layer

Krizhevsky, et al.
NIPS 4824





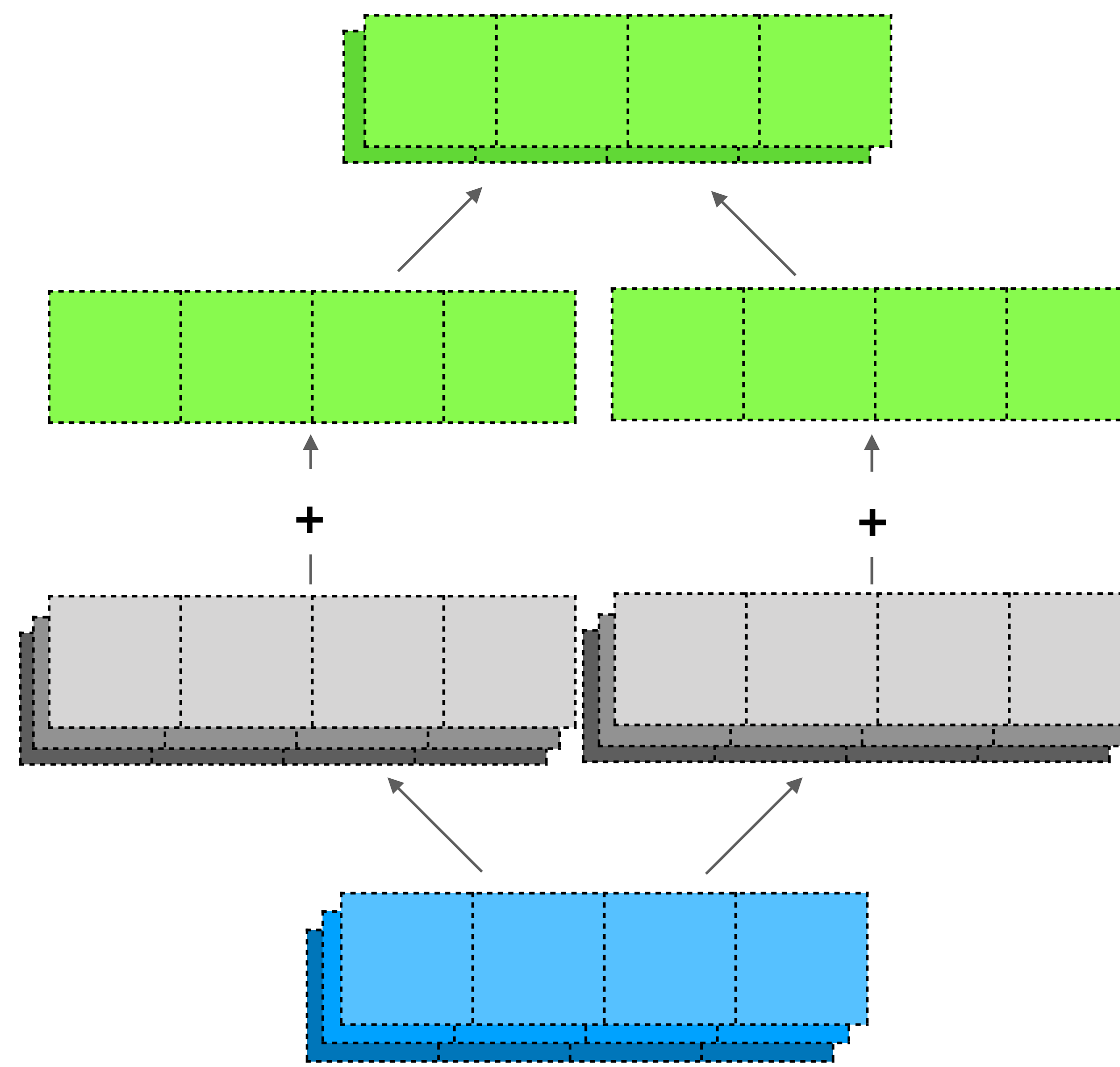
1D CONVOLUTIONAL LAYER



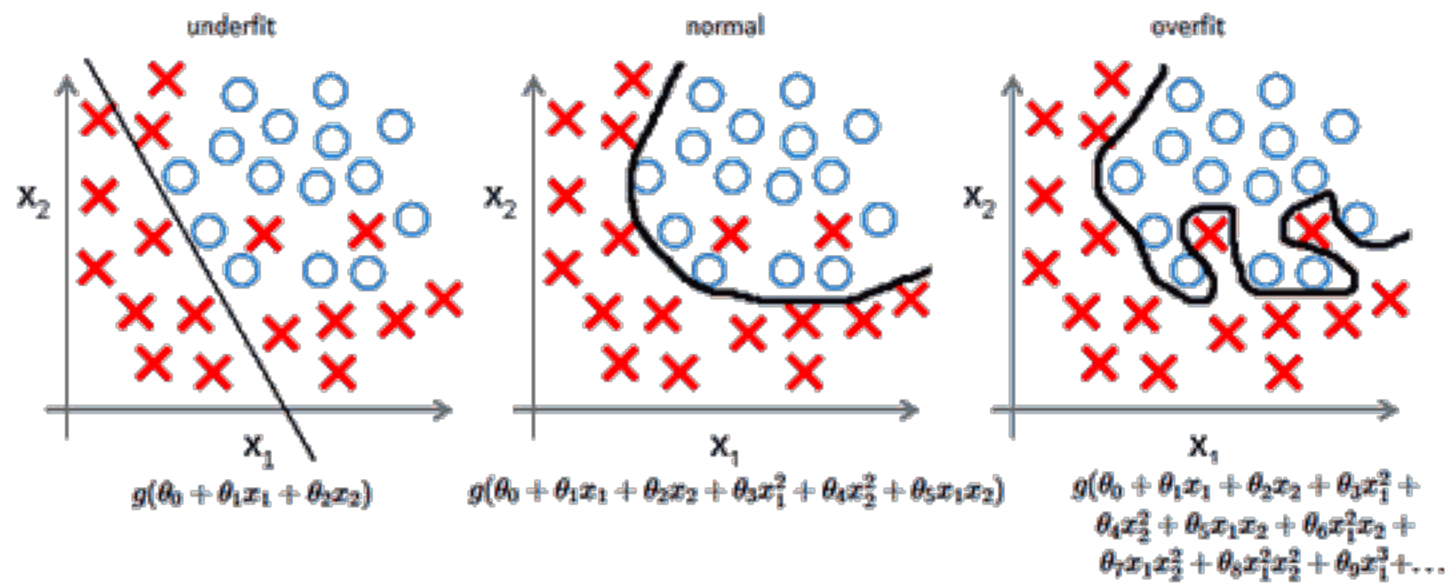
- Filter moves across input dimension

$$c_0 = f_0 i_{-1} + f_1 i_0 + f_2 i_1$$

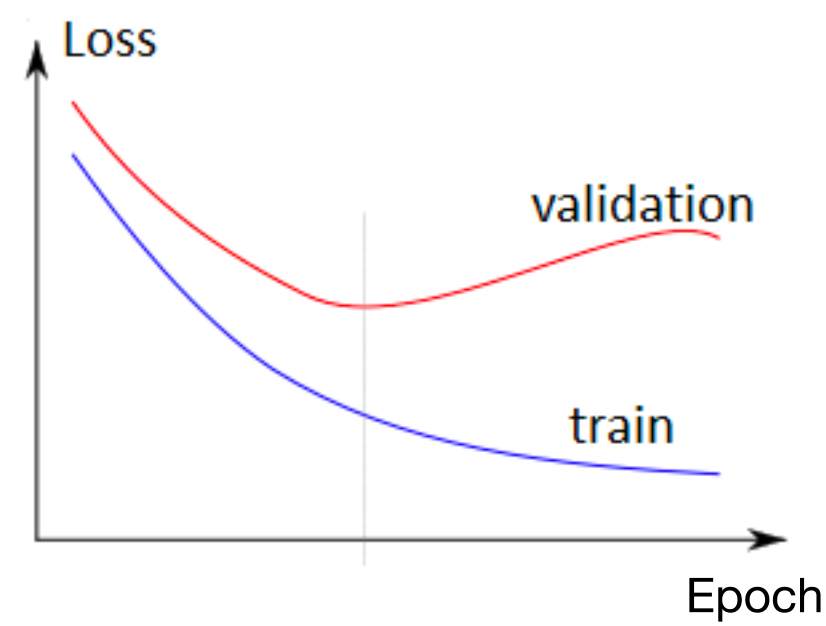
- Example hyper-parameter settings:
- Input size = 4
- Number of channels = 3
- Filter size = 3
- "Same" / "Half" zero padding
- Number of filters = 2
- Output size = 4



OVERFITTING

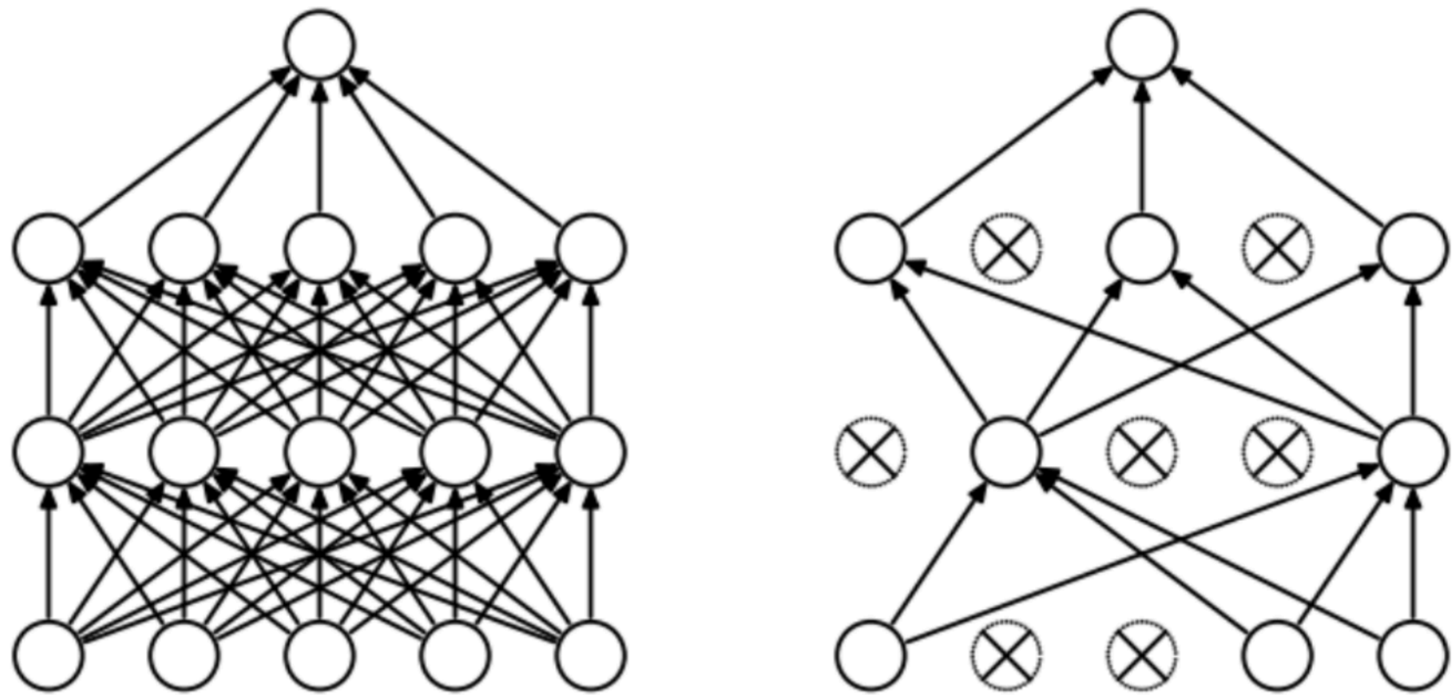


- Split data to training/validation/test sets:
  - After each *epoch* (one iteration of training on the whole dataset), validate the model on the validation set; stop training when overfitting appears
  - Benchmark final model on the test set



DROPOUT

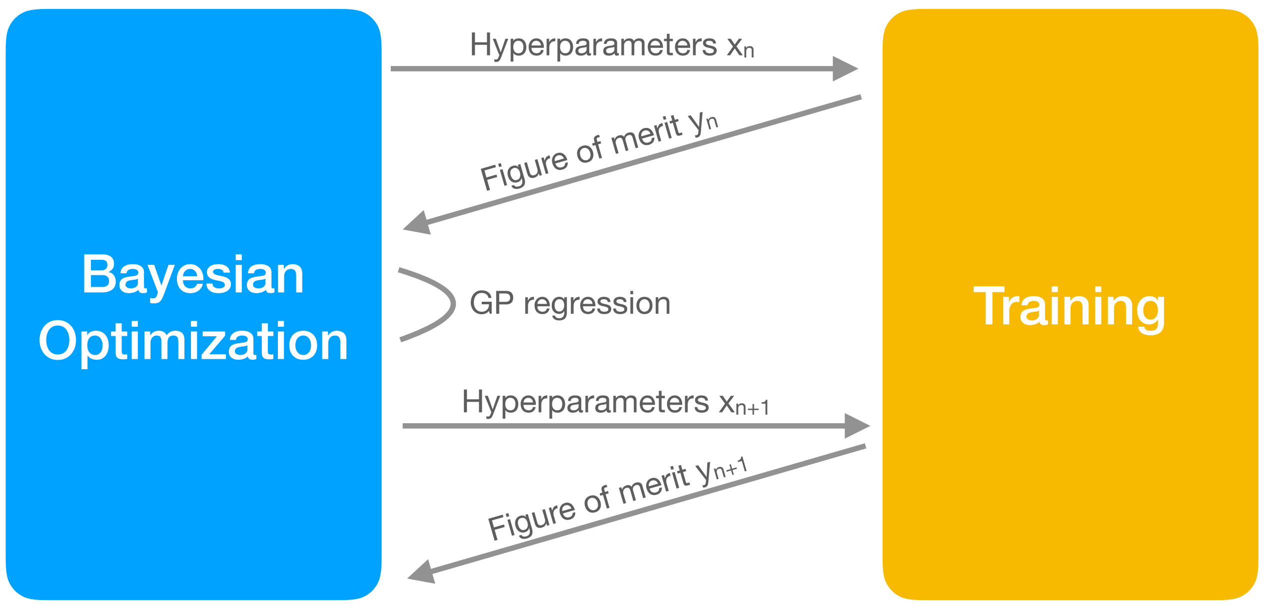
Srivastava et. al.

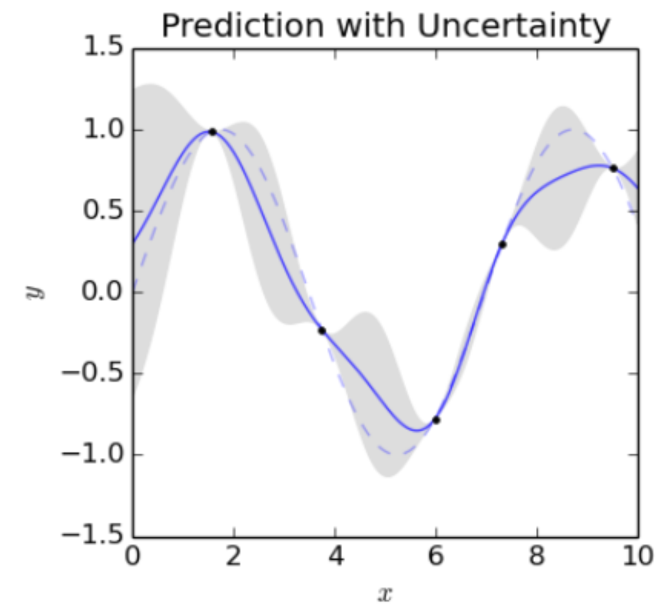


(a) Standard Neural Net (b) After applying dropout.

- Randomly remove connections between layers
- Effective against overfitting

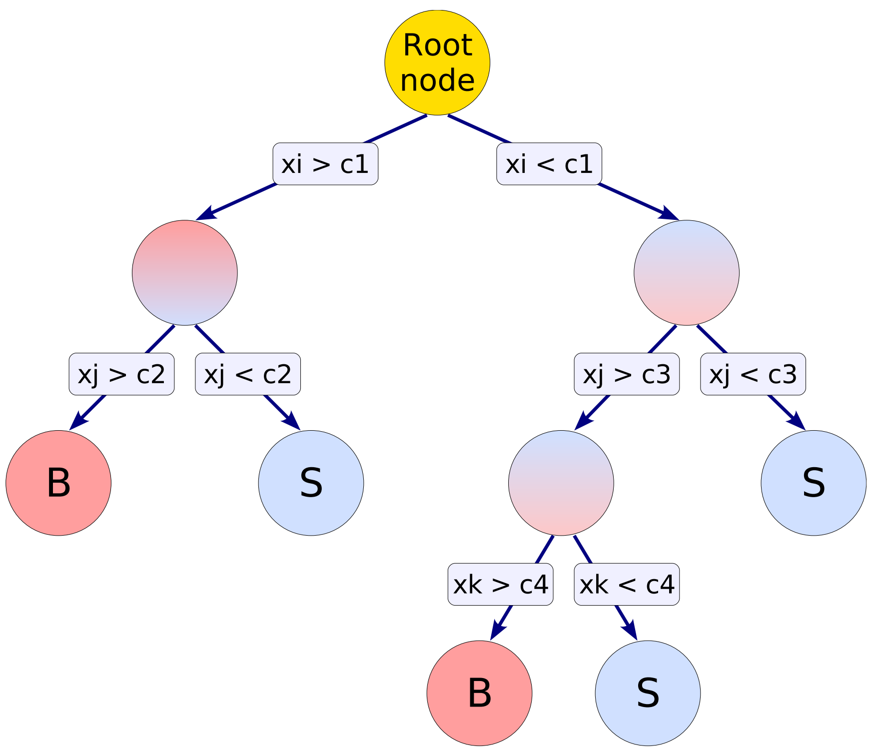
BAYESIAN OPTIMIZATION





- Objective: Find the optimal point in hyperparameter space x that minimizes the objective function y = f(x).
- Bayesian optimization: fit the distribution $\{y_n = f(x_n)\}_{n=1..N}$ with Gaussian process regression, predict the next value x_{N+1} that offers the best expected improvement on y.
- x = set of hyperparameters
- f(x) = final validation loss or negative validation accuracy of the model trained with given set of hyperparameters x

BOOSTED DECISION TREE



- Decision trees – can be seen as extension of cut-based selection
- Growing the tree: each cut determined by the variable and splitting value that give the best separation (Purity, Cross entropy, Gini coefficiet, etc.)
- Enhanced purity in leaves
- "Boosting"
  - A forest of decision trees, classify event based on majority votes of each tree
  - When growing new trees, greater weights given to previously misclassified events
  - For each new tree, its "voting weight" is set in such as way so as to minimize the total classification error of the forest
  - Most popular variant: Adaboost

DOMAIN ADVERSARIAL TRAINING

arXiv:1611.01046
arXiv:1409.7495

DOMAIN ADVERSARIAL TRAINING

arXiv:1611.01046
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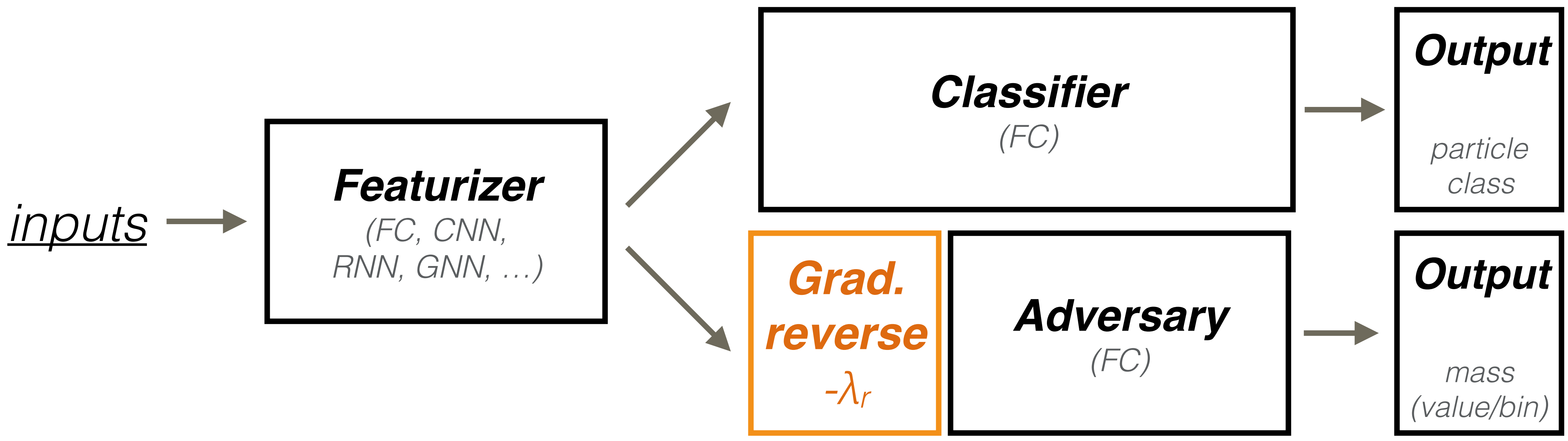
$$L = L_{\text{disc}} + \lambda L_{\text{adv}}$$



- Adversarial training: second neural network (adversary) trained against original network (classifier)

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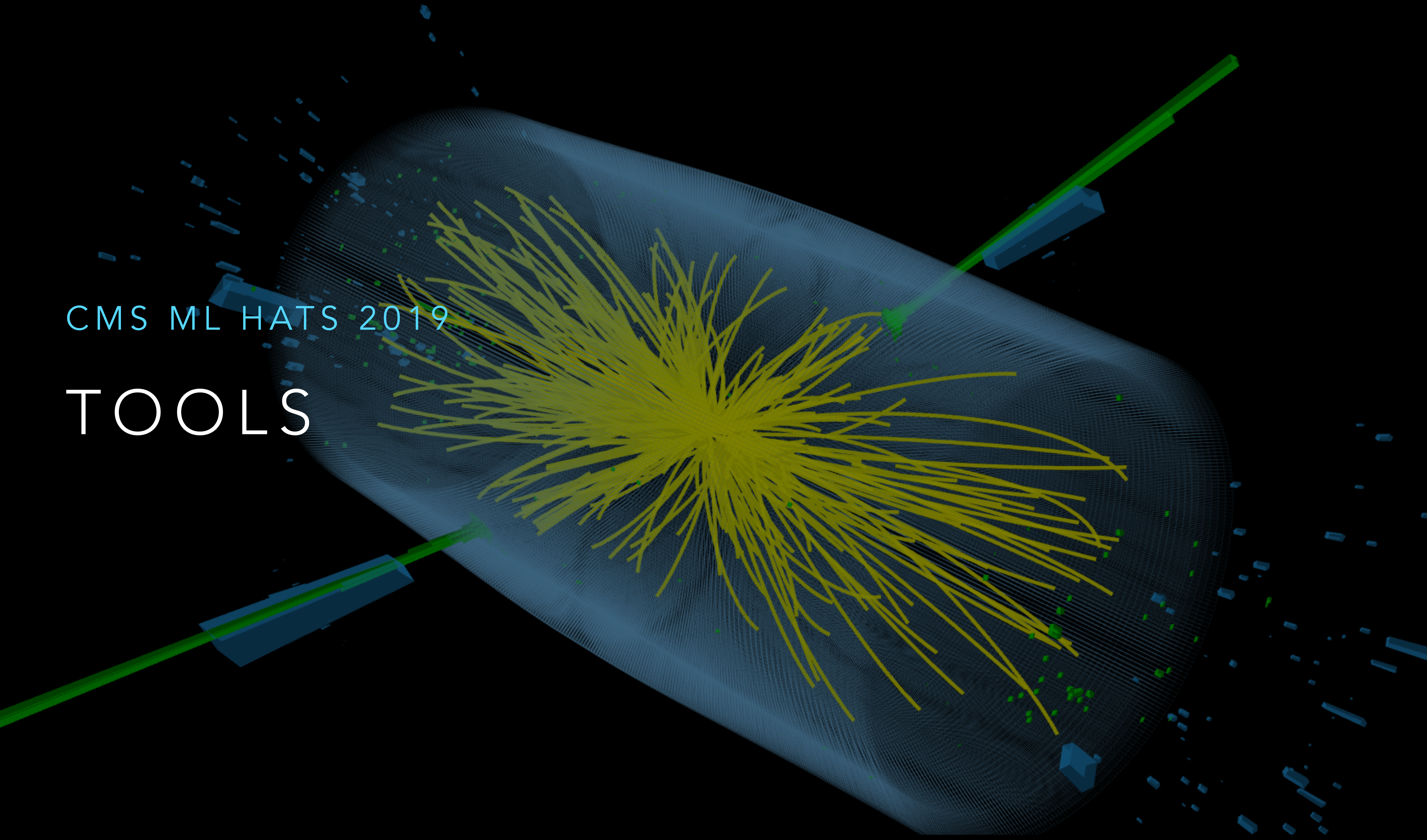
TOOLS



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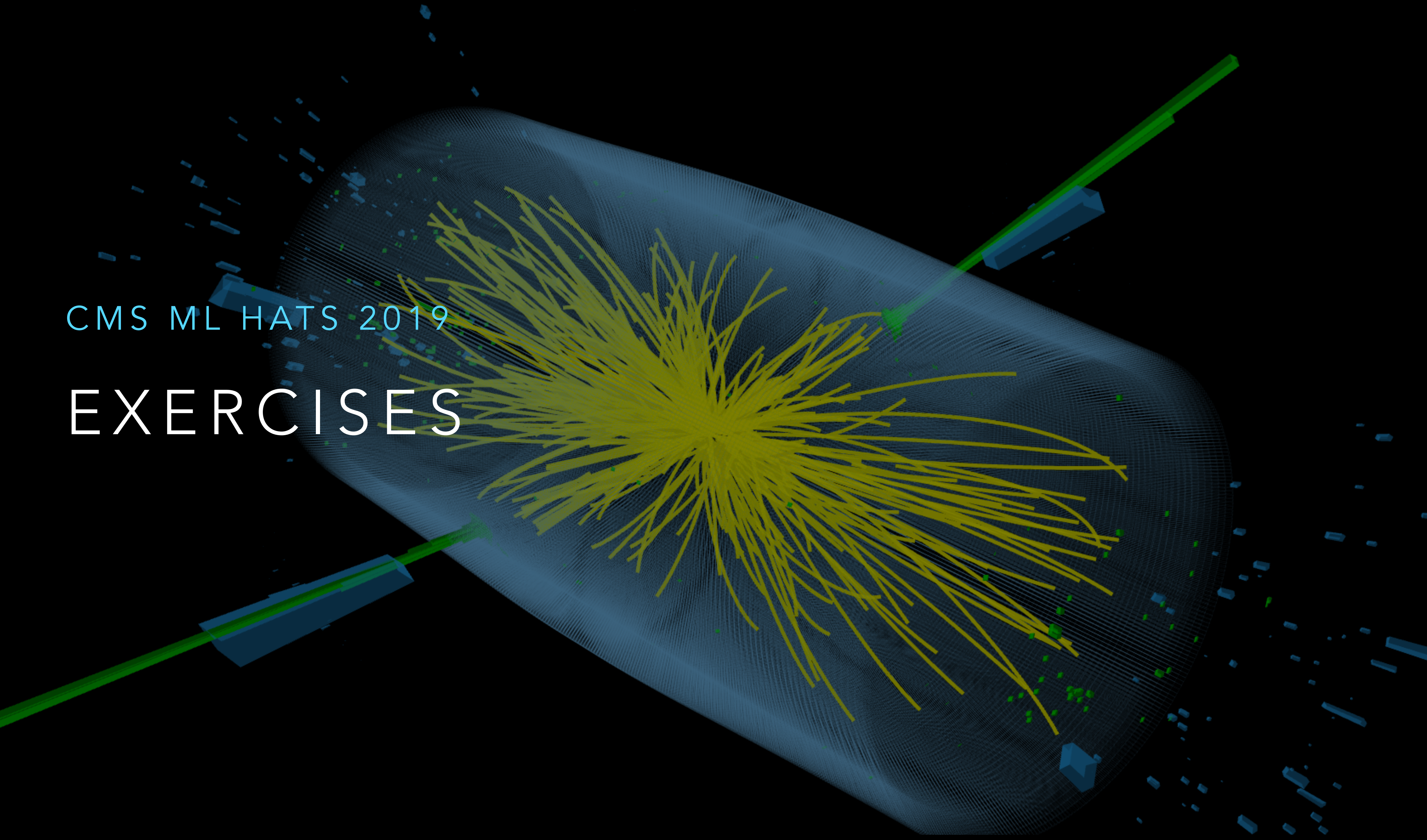
TOOLS

- Python
  - NumPy: http://www.numpy.org/
  - SciPy: https://www.scipy.org/
- Machine Learning
  - scikit-learn: http://scikit-learn.org/
  - Keras: https://keras.io/
  - PyTorch: https://pytorch.org/
- CMS/HEP
  - root_numpy: http://scikit-hep.org/root_numpy/
  - uproot: https://github.com/scikit-hep/uproot
  - DL4Jets/DeepJet: https://github.com/DL4Jets/DeepJet



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EXERCISES

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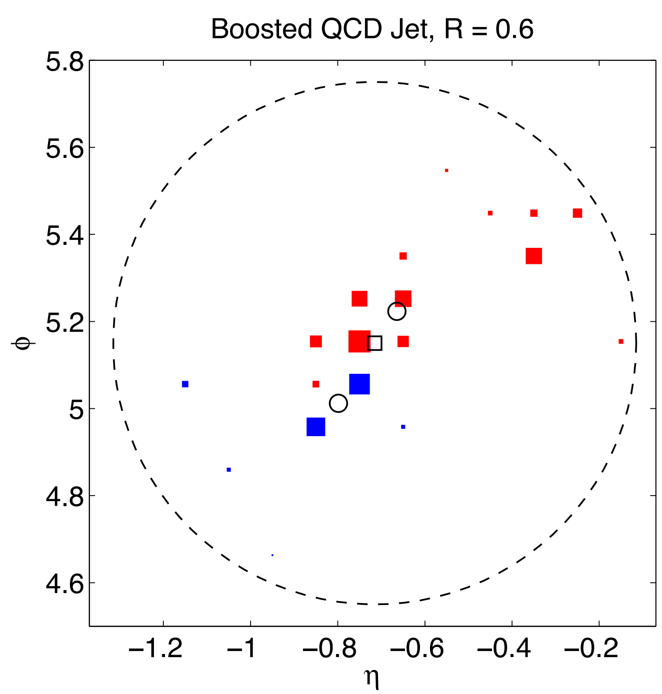
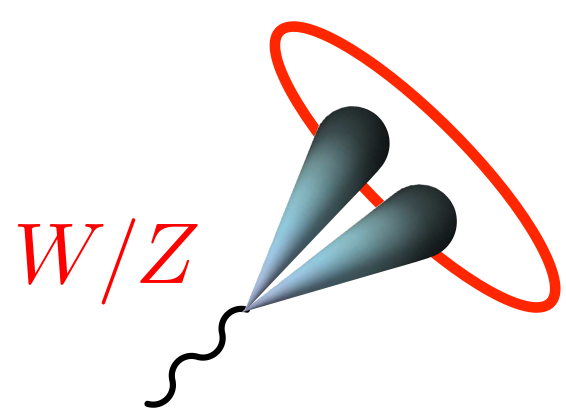
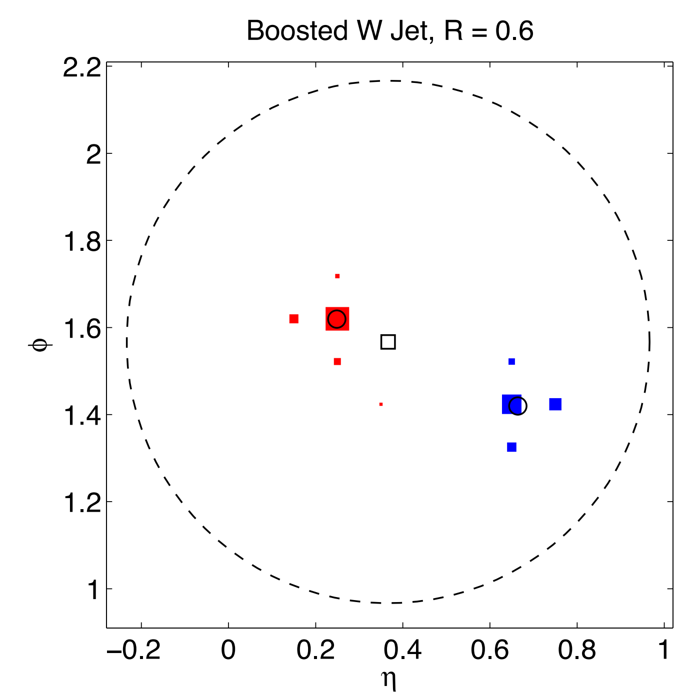
CLASSIC JET PROBLEM

- A jet is a collimated spray of energetic particles originating from the fragmentation of scattered partons (quarks or gluons)
- One classic problem is identifying whether the jet originates from the decay of a boosted particle W/Z/H/t or simply from a quark/gluon (QCD)





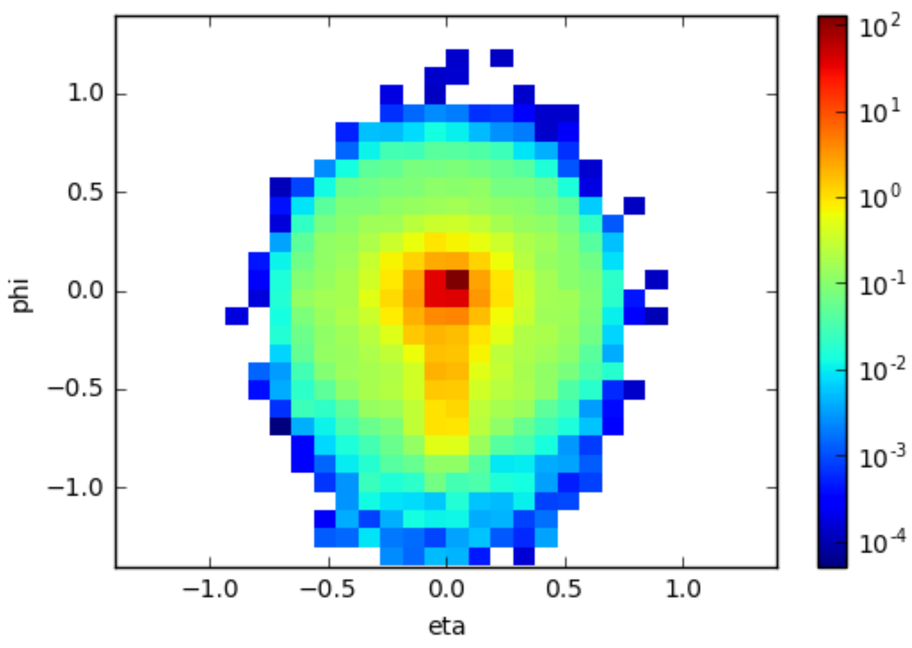


[J. Thaler, et al. arXiv:1011.2268]

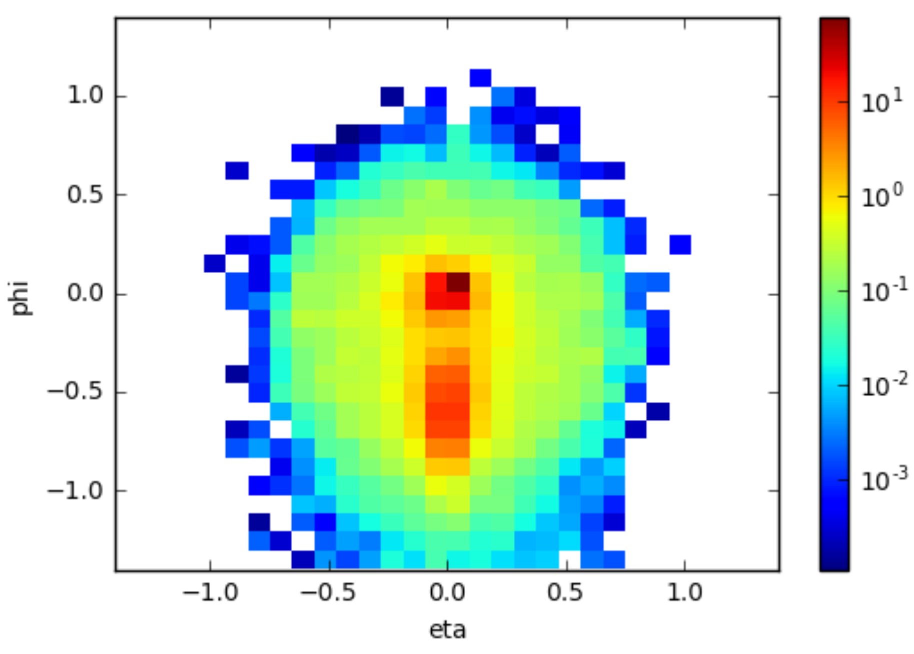
JET-IMAGES

- Visualize jets as an discrete images
- Note: these are averaged images!

QCD mean jet image



W jet image



DATASET LOCATION

- Available on CMS LPC: root://cmseos.fnal.gov//eos/uscms/store/user/woodson/DSHEP2017/
- Small subset available on CERNBox: https://cernbox.cern.ch/index.php/s/NTG4OgGik4rIsOk

REFERENCES

- A high-bias, low-variance introduction to machine learning for physicists: https://arxiv.org/abs/1803.08823
- Michael Kagan. CERN Academic Lectures on Machine Learning: https://indico.cern.ch/event/619370/
- Yisong Yue. Caltech Machine Learning & Data Mining cosrse: http://www.yisongyue.com/courses/cs155/2018_winter/

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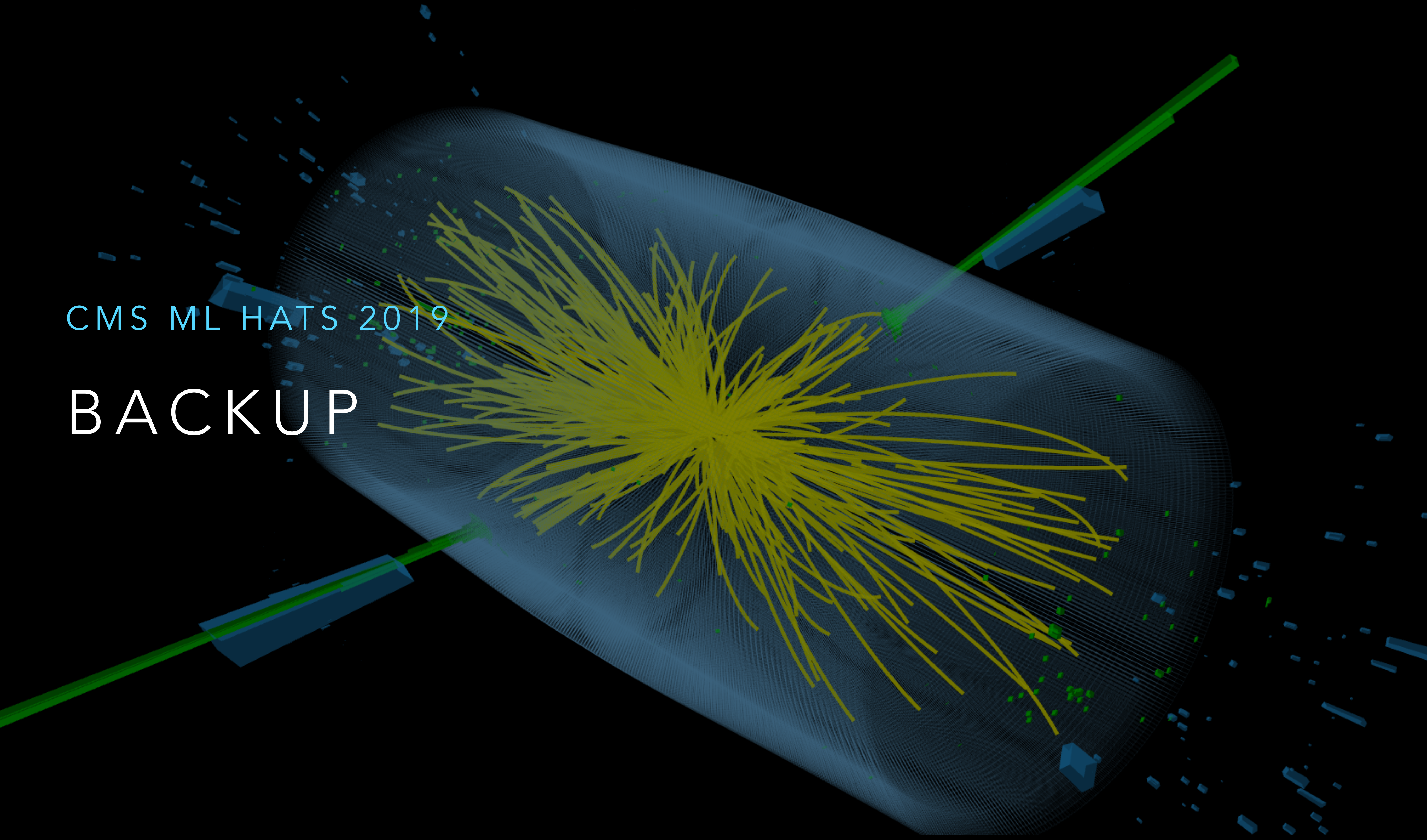
BACKUP



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