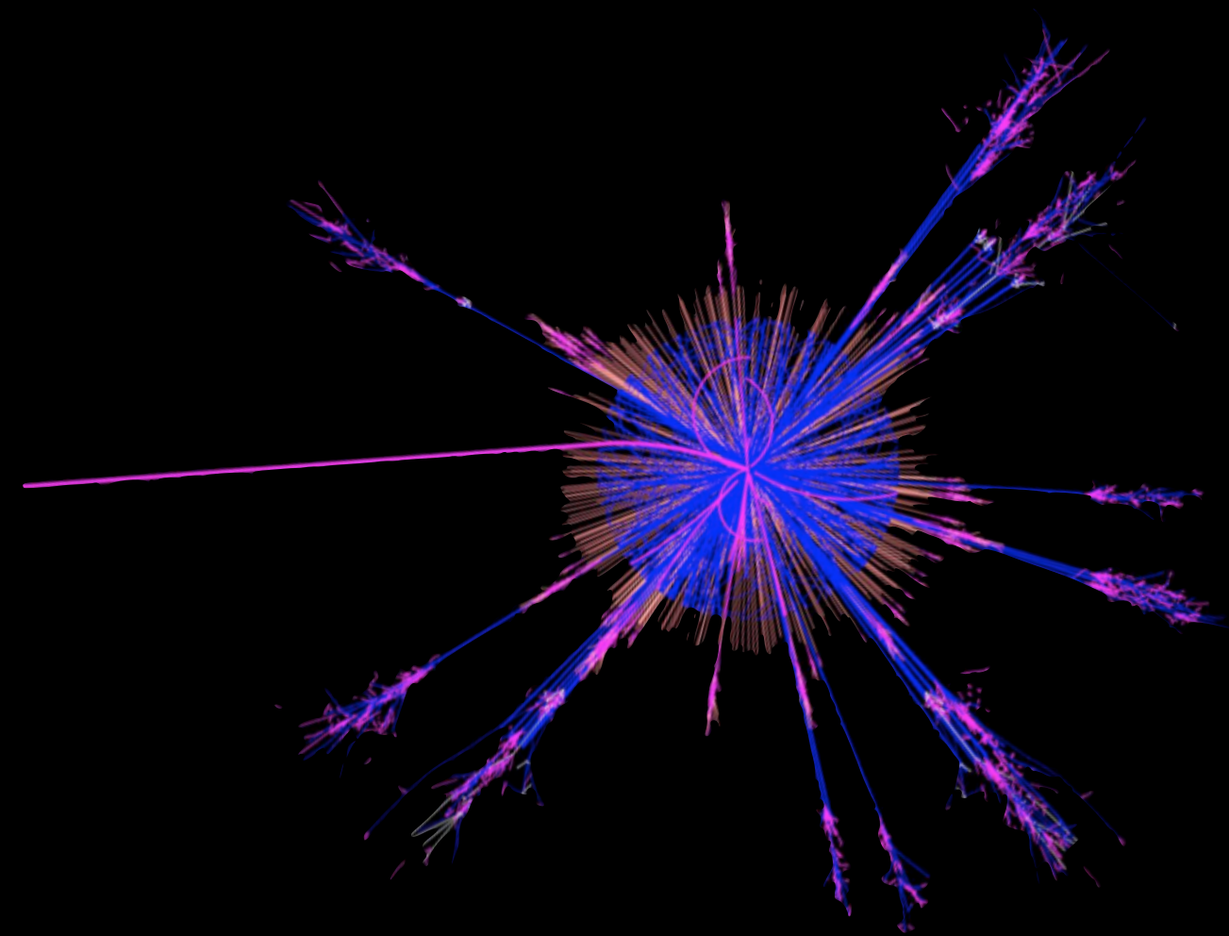
NYU Center for Data Science

Center for Cosmology and Particle Physics

MISCELLANEOUS THOUGHTS ON

ML & DM



@KyleCranmer
New York University
Department of Physics
Center for Data Science
CILVR Lab

HOW DO WE WANT ML TO HELP?

More powerful searches

More robust searches in face of large uncertainties

- data-driven vs. simulation-based

Difficult Inverse problems

- eg. weak lensing, strong lensing; indirect detection

Interpretation of results & decision making

- speed up the inference pipeline
- improve decisions based on current knowledge

Deep Learning for Physical Sciences

Workshop at the 31st Conference on Neural Information Processing Systems (NIPS)

December 8, 2017

THE PLAYERS

forward modeling
generation
simulation

PREDICTION

θ
parameters of interest

$p(x, z \mid \theta, \nu)$

x
observed data
simulated data

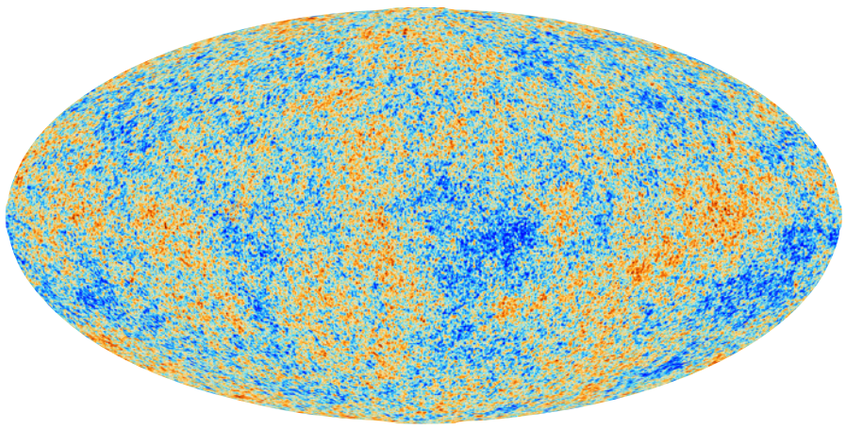
z
latent variables
Monte Carlo truth

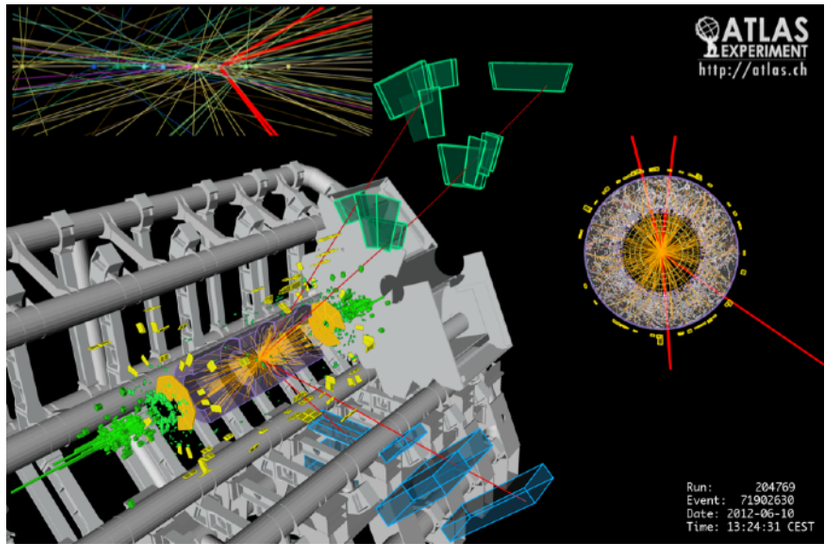
ν
nuisance parameters

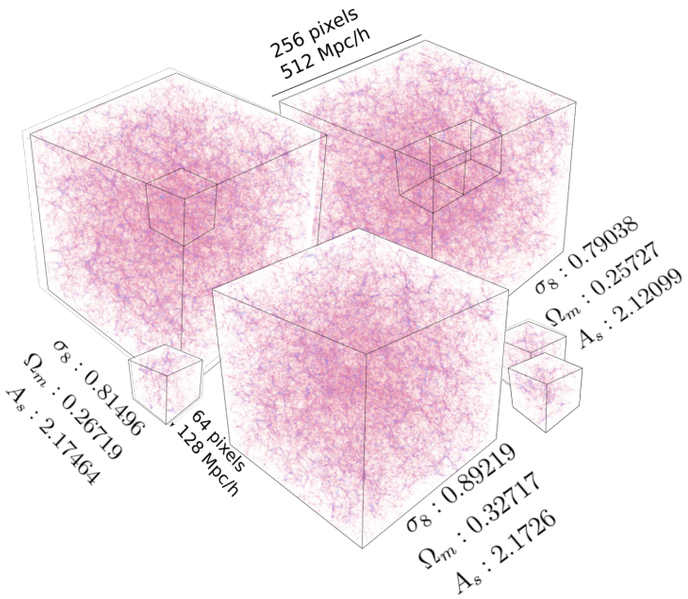
INFERENCE

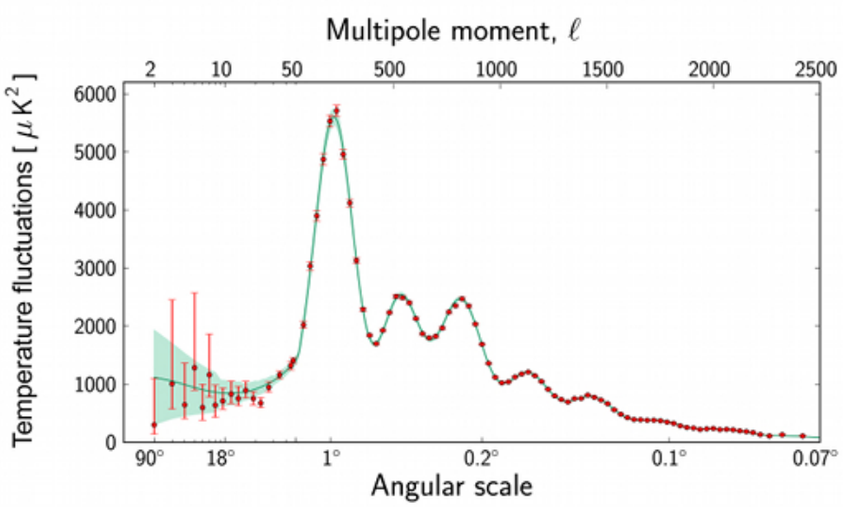
inverse problem
measurement
parameter estimation

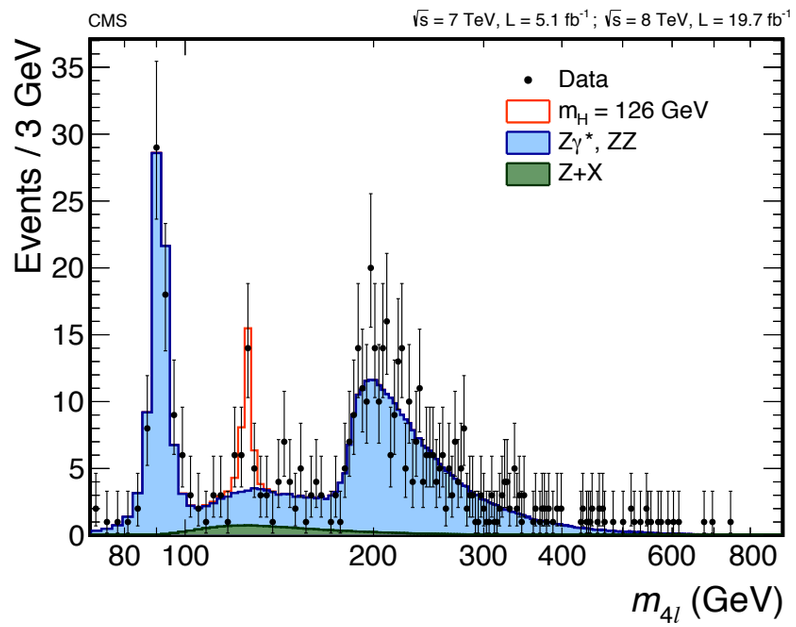
PREDICTION: THE FORWARD MODEL

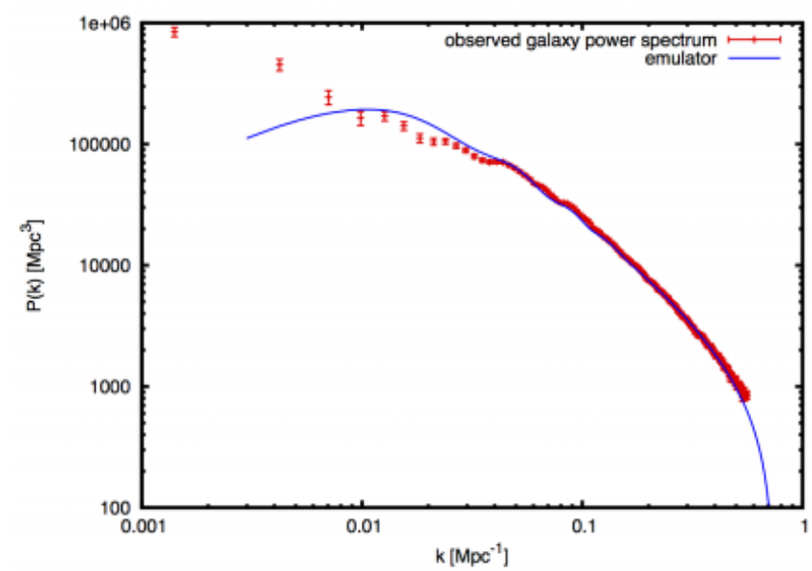












WHY WE SHOULD CARE

Many areas of science have simulations based on some well-motivated mechanistic model.

However, the aggregate effect of many interactions between these low-level components leads to an intractable inverse problem.

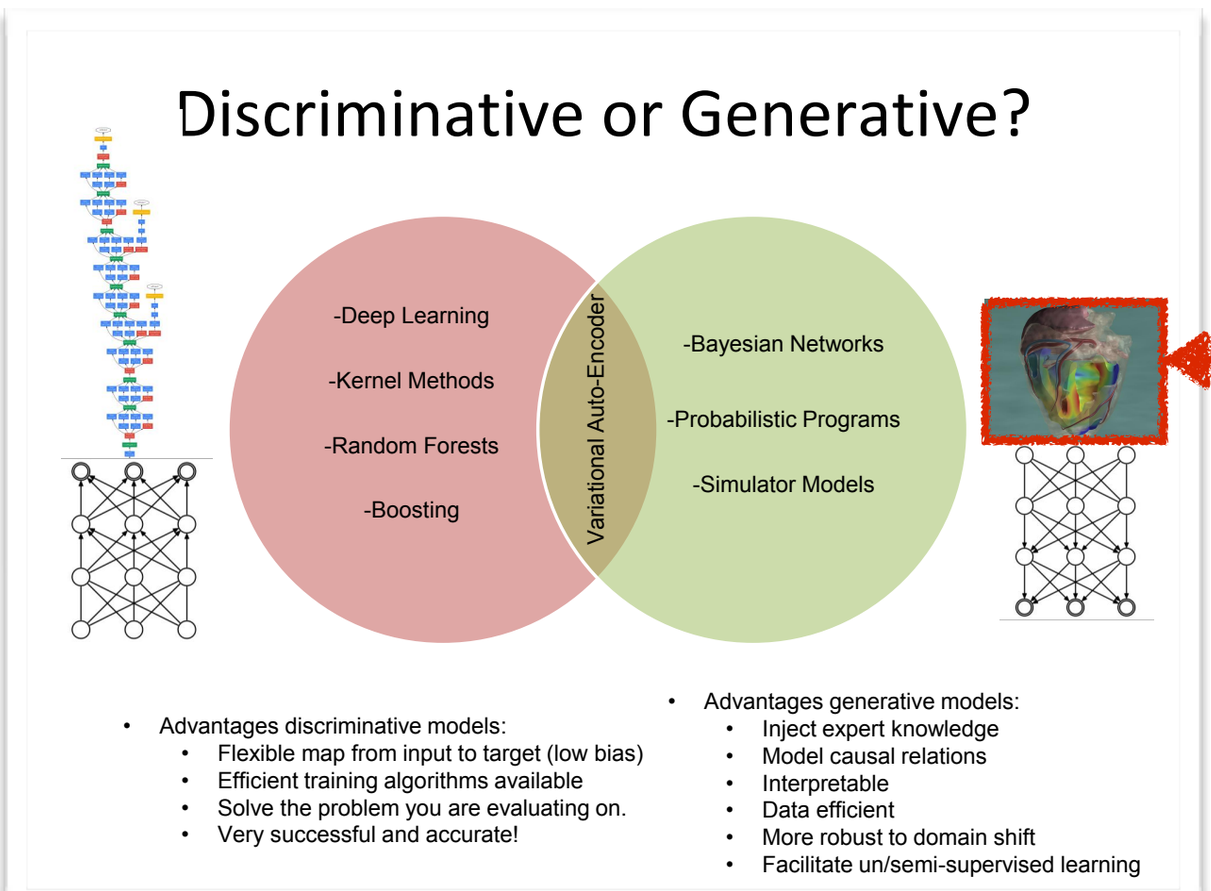
The developments in machine learning and AI go way beyond improved classifiers and have the potential to effectively bridge the microscopic - macroscopic divide & aid in the inverse problem.

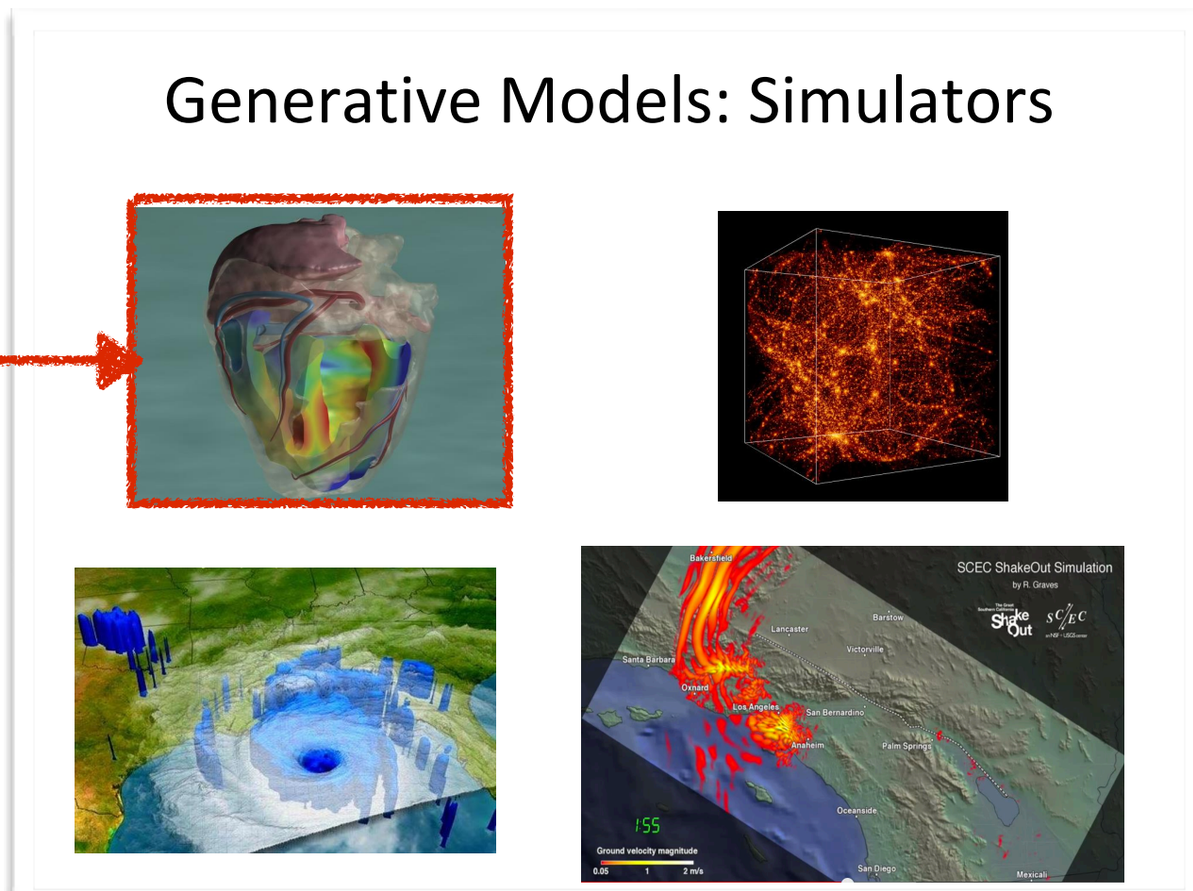
- they can provide effective statistical models that describe macroscopic phenomena that are tied back to the low-level microscopic (reductionist) model
- generative models and likelihood-free inference are two particularly exciting areas

FROM MAX'S TALK

The image of the heart represents a simulator (yes, there are heart simulators!)

The heart is also represented on the generative side of the machine learning dichoticomy.





COLLIDER PHYSICS VS. DM

Collider physics has a very good simulator for the data, backgrounds are well understood

- good setting for supervised learning & discriminative models

In contrast, many search strategies for DM have uncertain nuclear physics or astrophysical backgrounds. Need to be data driven!

- weakly supervised
- unsupervised

Comment: Deep Learning isn't necessarily the best for dealing with large uncertainties. More natural with Gaussian Processes, Bayesian Neural Networks, probabilistic programs, etc.

Lesson

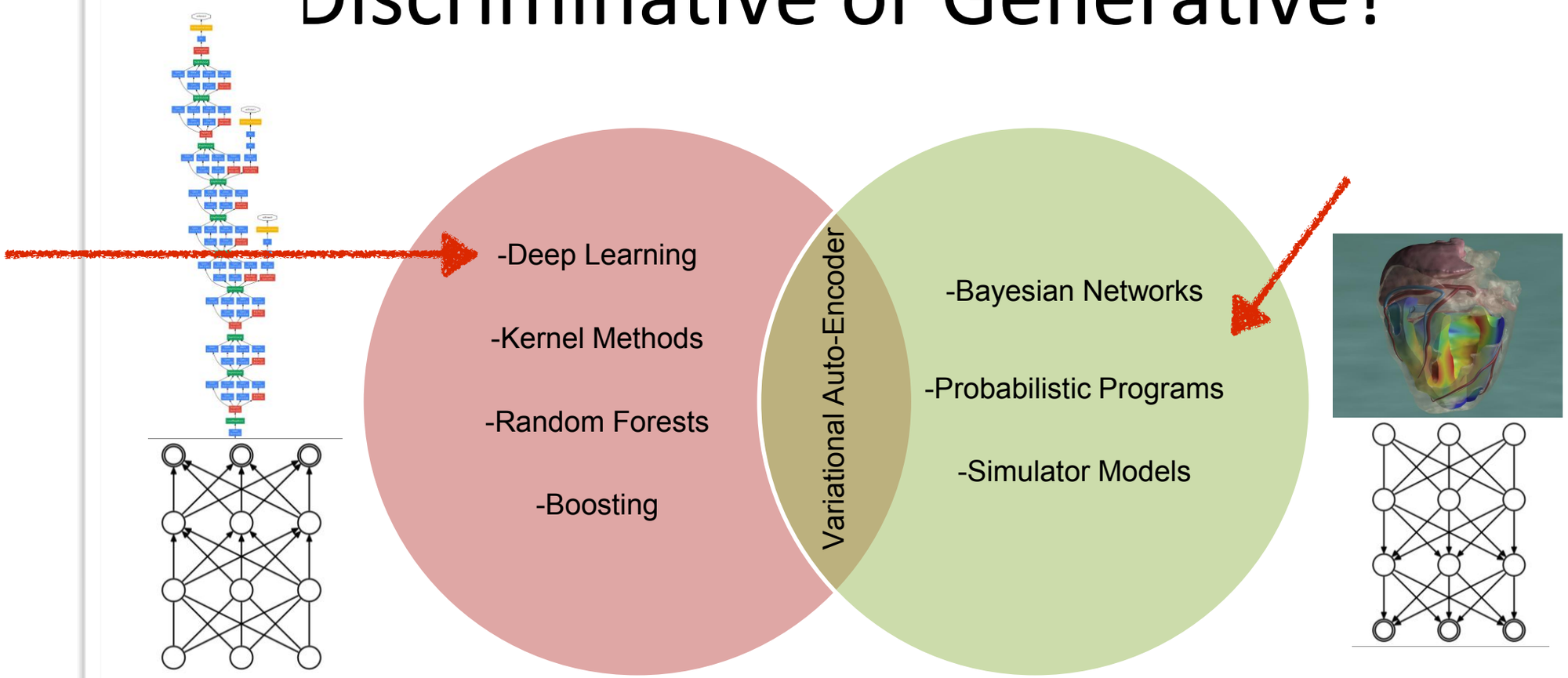
We have been discovering new properties of the "backgrounds" as we try to discover DM

→ "Backgrounds" are known up to an O(1) factor.

Supervised vs unsupervised algorithm?
Deep learning is mandatory, but is it enough?

Many DM problems need advantages of generative models

Discriminative or Generative?



- Advantages discriminative models:
  - Flexible map from input to target (low bias)
  - Efficient training algorithms available
  - Solve the problem you are evaluating on.
  - Very successful and accurate!

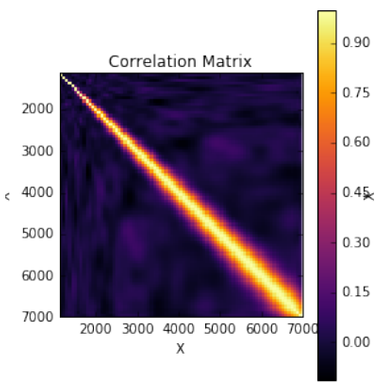
- Advantages generative models:
  - Inject expert knowledge
  - Model causal relations
  - Interpretable
  - Data efficient
  - More robust to domain shift
  - Facilitate un/semi-supervised learning

PHYSICS-AWARE MACHINE LEARNING

Not easy, but there are ways of injecting physics knowledge into discriminative models as well…

Physics-aware Gaussian Processes

arXiv:1709.05681

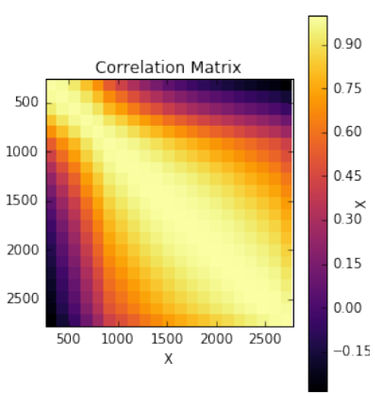


Final Kernel =

Poisson fluctuations

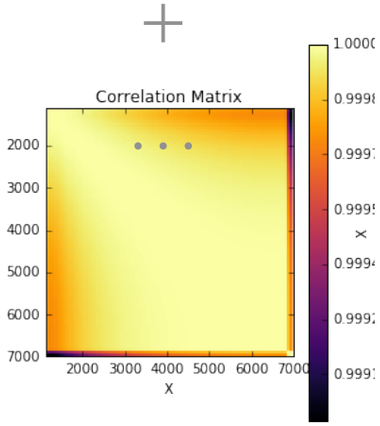
=

+ Mass Resolution



+ Parton Density Functions

+

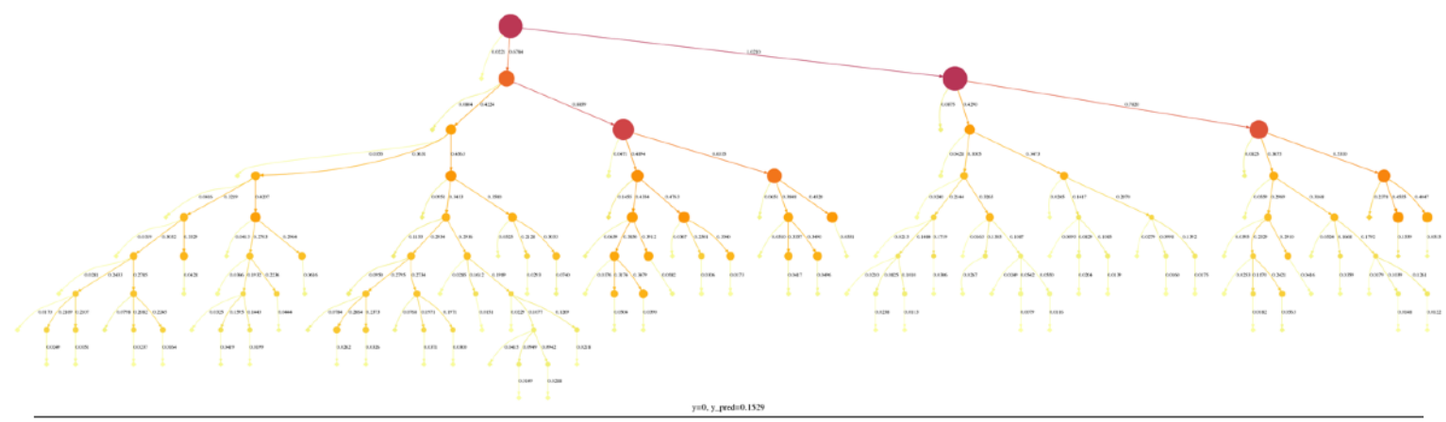


+ Jet Energy Scale

+

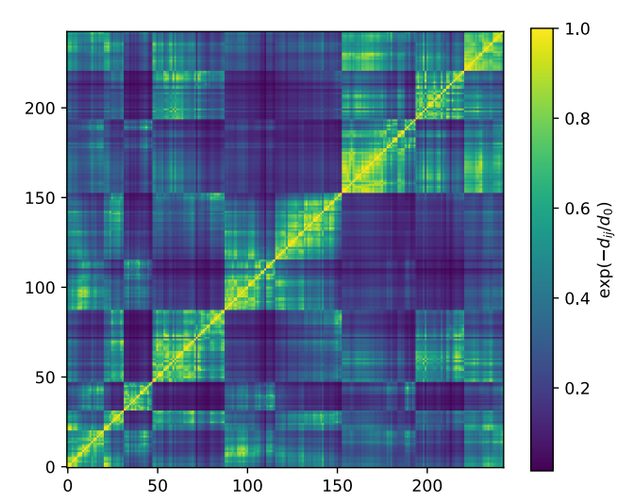
QCD-Aware recursive neural networks

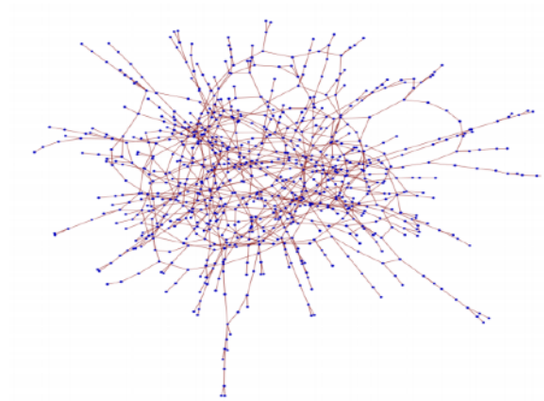
arXiv:1702.00748



QCD-Aware graph convolutional neural networks

NIPS2017 workshop [http://bit.ly/2AkwYRG]

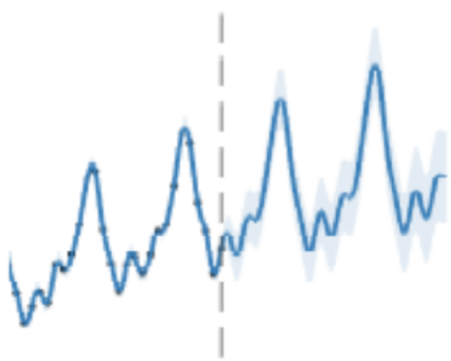




$$d^{\alpha}_{ii'} = \min(p^{2\alpha}_{ti}, p^{2\alpha}_{ti'}) \frac{\Delta R^2_{ii'}}{R^2}$$

Vocabulary of kernels + grammar for composition

- physics goes into the construction of a "Kernel" that describes covariance of data

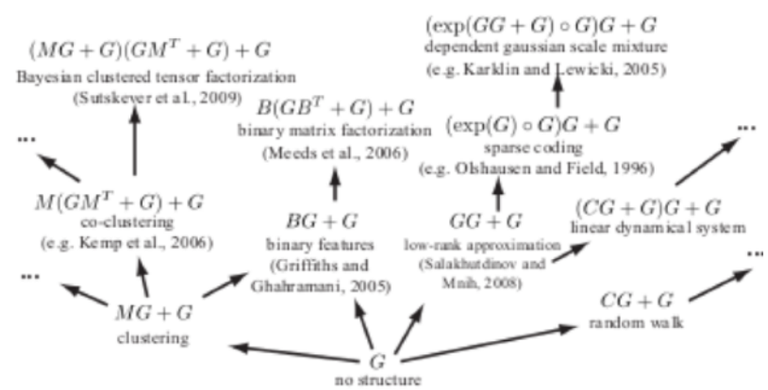


Structure Discovery in Nonparametric Regression through Compositional Kernel Search

David Duvenaud, James Robert Lloyd, Roger Grosse, Joshua B. Tenenbaum, Zoubin Ghahramani

International Conference on Machine Learning, 2013

pdf | code | poster | bibtex



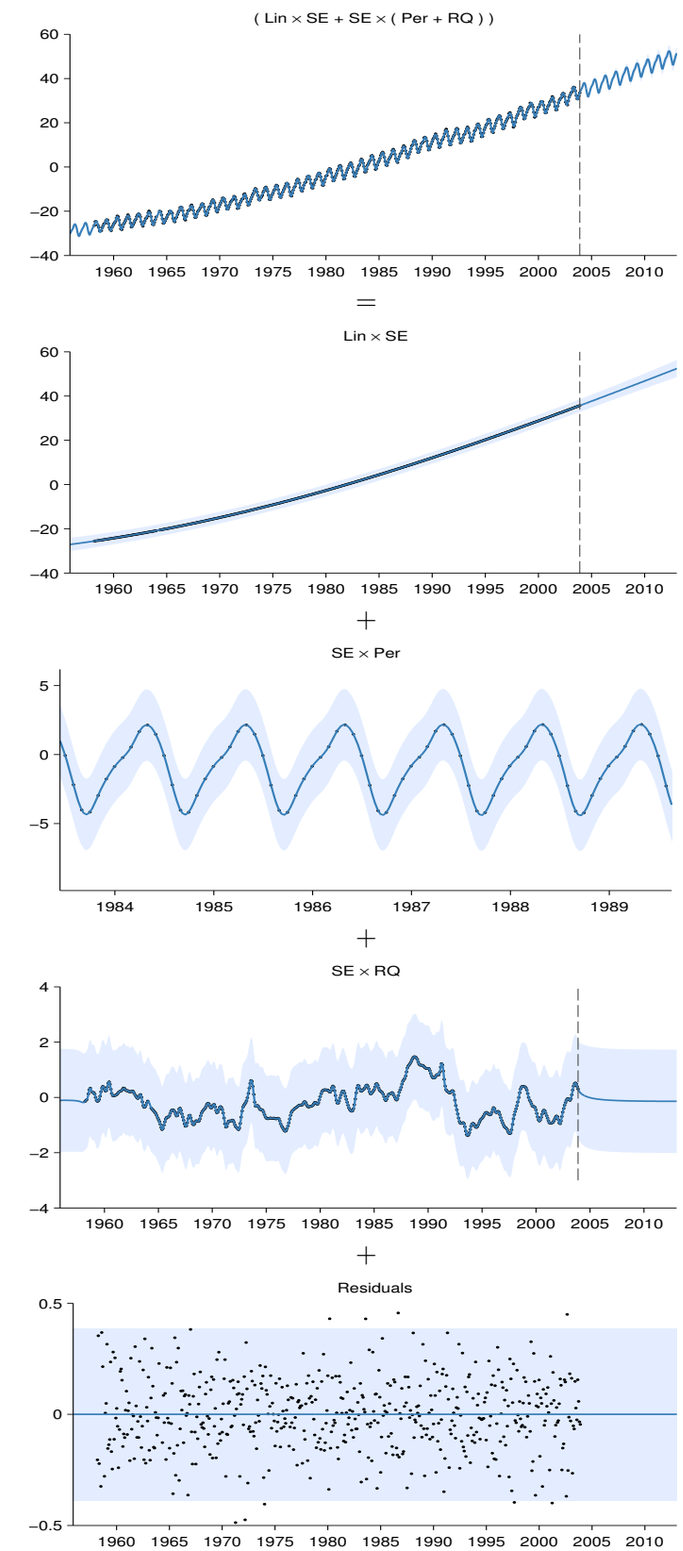
Exploiting compositionality to explore a large space of model structures

Roger Grosse, Ruslan Salakhutdinov, William T. Freeman, Joshua B. Tenenbaum

Conference on Uncertainty in Artificial Intelligence, 2012

pdf | code | bibtex

Mauna Loa atmospheric CO_2



Discriminative Models:

Training them with Real Data Using Weakly Supervised Learning

TRAINING ON DATA WITH WEAKLY SUPERVISED

Classification without labels:
Learning from mixed samples in high energy physics

Eric M. Metodiev,[a] Benjamin Nachman,[b] and Jesse Thaler[a]

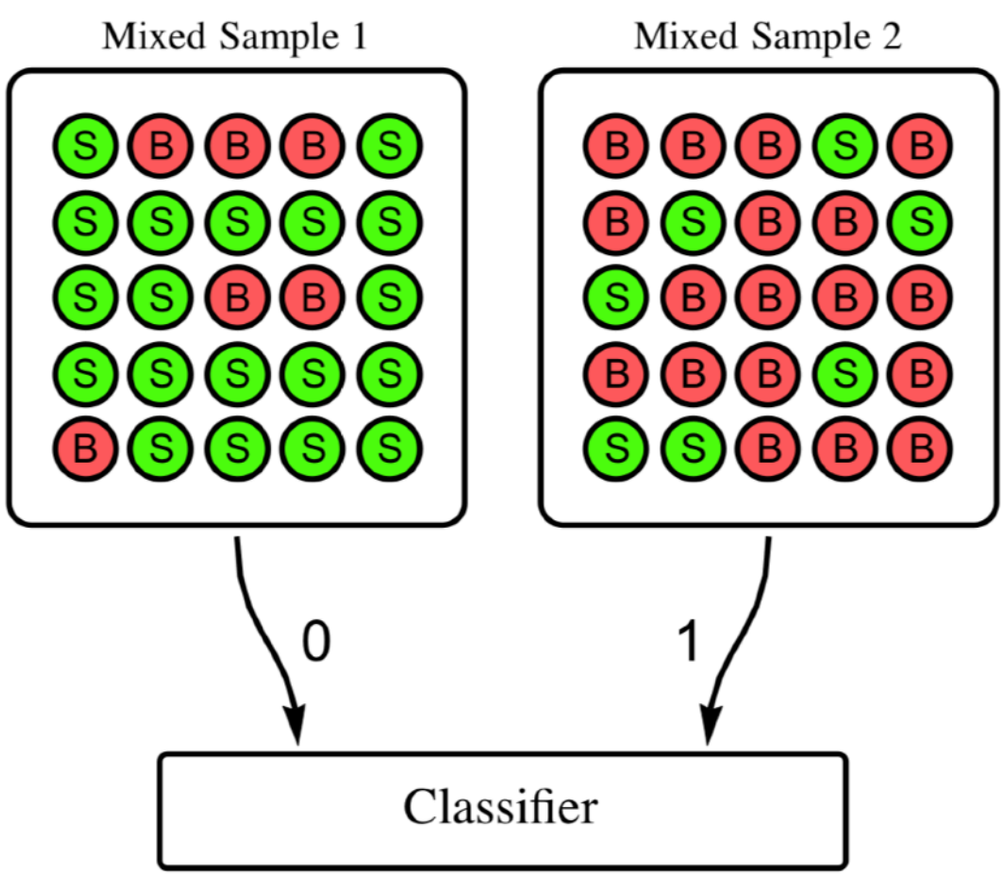
[a] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[b] *Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

E-mail: metodiev@mit.edu, bpnachman@lbl.gov, jthaler@mit.edu

Weakly Supervised Classification in High Energy Physics

Lucio Mwinmaarong Dery[a] Benjamin Nachman[b] Francesco Rubbo[c] Ariel Schwartzman[c]

[a] *Physics Department, Stanford University, Stanford, CA, 94305, USA*
[b] *Physics Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA, 94720, USA*
[c] *SLAC National Accelerator Laboratory, Stanford University, 2575 Sand Hill Rd, Menlo Park, CA, 94025, USA*
E-mail: ldery@slac.stanford.edu, bnachman@cern.ch, rubbo@slac.stanford.edu, sch@slac.stanford.edu



Possible to learn classifier between "signal" and "background" from real (unlabeled) data if:

- different samples with known class label proportions
- samples with unknown (but different) class label proportions

Requirement:

- distributions for different classes unaffected by selection effects

TRAINING ON DATA WITH WEAKLY SUPERVISED

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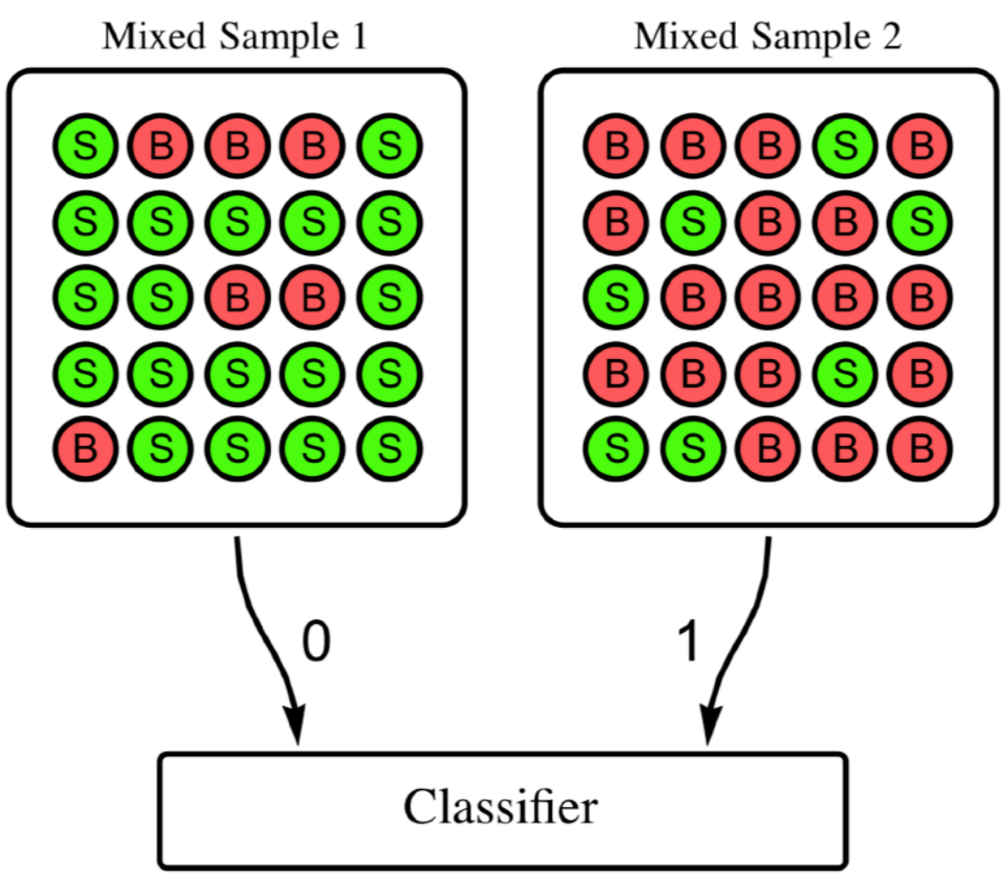


Direct detection:

- change calibration sources, shielding, etc. to modify proportions of signal-like and various backgrounds

Indirect detection

- can you use morphology or photon statistics as a handle to modify proportions of different populations?

Can you do this while maintaining requirements

LEARNING TO PIVOT

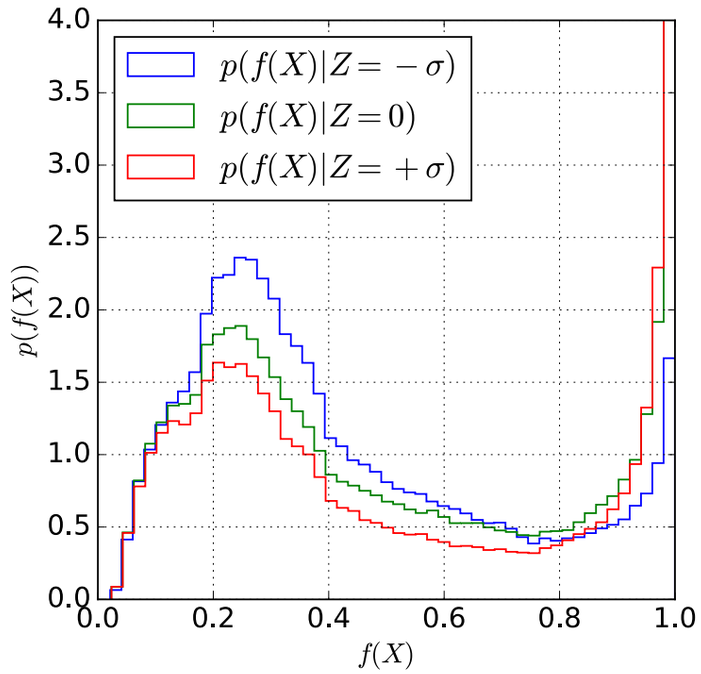
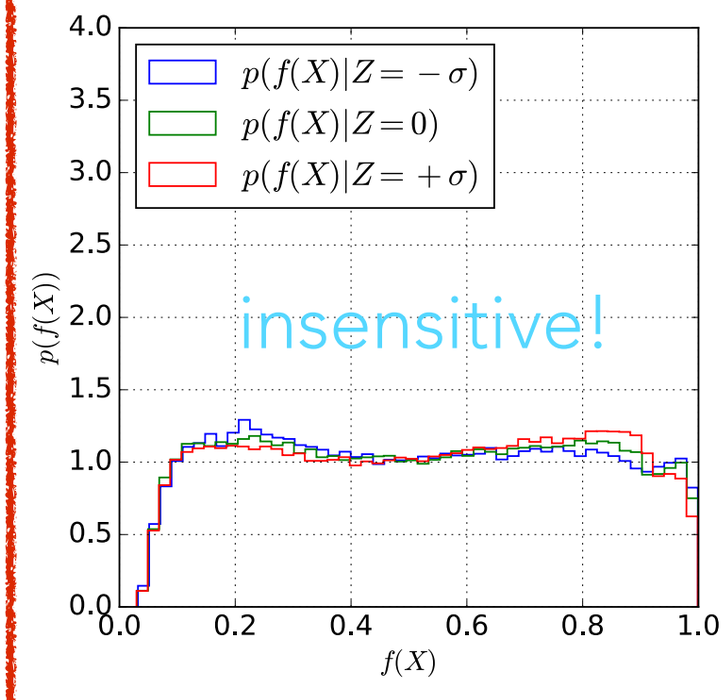
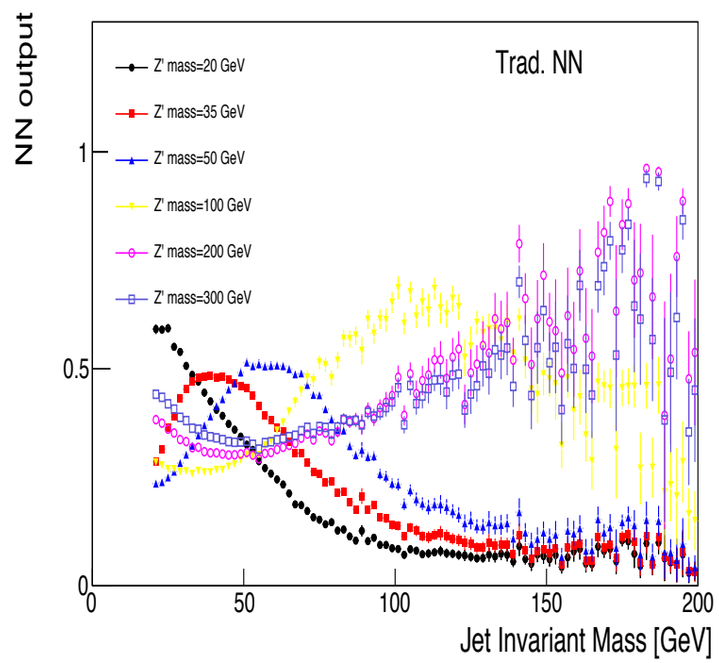
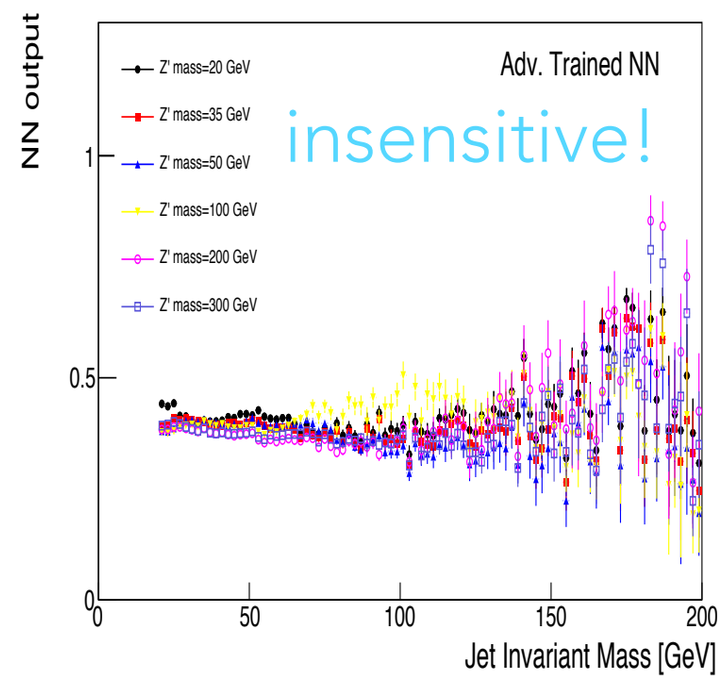
Tomorrow **Gilles Louppe** will talk about **Adversarial Games** including our work on "Learning to Pivot"

- Here network prediction is trained to be invariant to:
  - a nuisance parameter or some other observed variable
  - eg. a classifier that is robust to systematics or independent of some variable

Can combine learning to pivot with weakly supervised techniques.

- **If** selection requirements affect the distributions
- **and** you either know what variables in selection are responsible for biasing the distributions or you have a model for with nuisance parameters describing uncertainty in how those distributions are affected
- **then** you can train classifier to be invariant to those variables or nuisance parameters, thus incorporating systematic uncertainty

LEARNING TO PIVOT

	Normal Training	Adversarial Training
Nuisance Parameter		
Other Variable		

Generative Modeling

ICML 2017 Workshop on Implicit Models

Workshop Aims

Probabilistic models are an important tool in machine learning. They form the basis for models that generate realistic data, uncover hidden structure, and make predictions. Traditionally, probabilistic models in machine learning have focused on prescribed models. Prescribed models specify a joint density over observed and hidden variables that can be easily evaluated. The requirement of a tractable density simplifies their learning but limits their flexibility --- several real world phenomena are better described by simulators that do not admit a tractable density. Probabilistic models defined only via the simulations they produce are called implicit models.

Arguably starting with generative adversarial networks, research on implicit models in machine learning has exploded in recent years. This workshop's aim is to foster a discussion around the recent developments and future directions of implicit models.

Implicit models have many applications. They are used in ecology where models simulate animal populations over time; they are used in phylogeny, where simulations produce hypothetical ancestry trees; they are used in physics to generate particle simulations for high energy processes. Recently, implicit models have been used to improve the state-of-the-art in image and content generation. Part of the workshop's focus is to discuss the commonalities among applications of implicit models.

Of particular interest at this workshop is to unite fields that work on implicit models. For example:

- **Generative adversarial networks** (a NIPS 2016 workshop) are implicit models with an adversarial training scheme.
- Recent advances in **variational inference** (a NIPS 2015 and 2016 workshop) have leveraged implicit models for more accurate approximations.
- **Approximate Bayesian computation** (a NIPS 2015 workshop) focuses on posterior inference for models with implicit likelihoods.
- Learning implicit models is deeply connected to **two sample testing, density ratio and density difference** estimation.

We hope to bring together these different views on implicit models, identifying their core challenges and combining their innovations.

If you have a generative model for the data

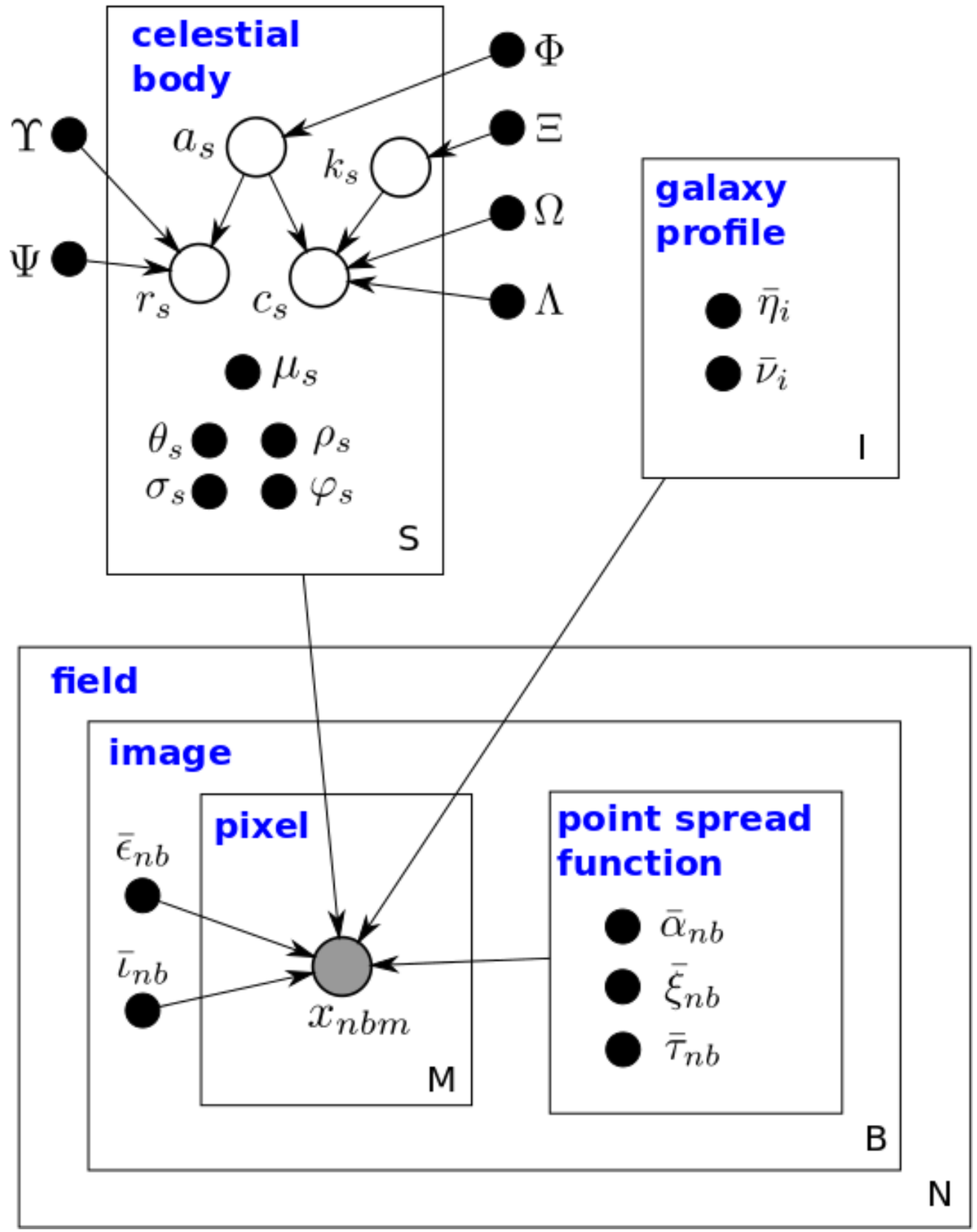
And you can evaluate likelihood

Then Variational Inference is a good fit

- A form of Machine Learning

- Able to inject expert knowledge

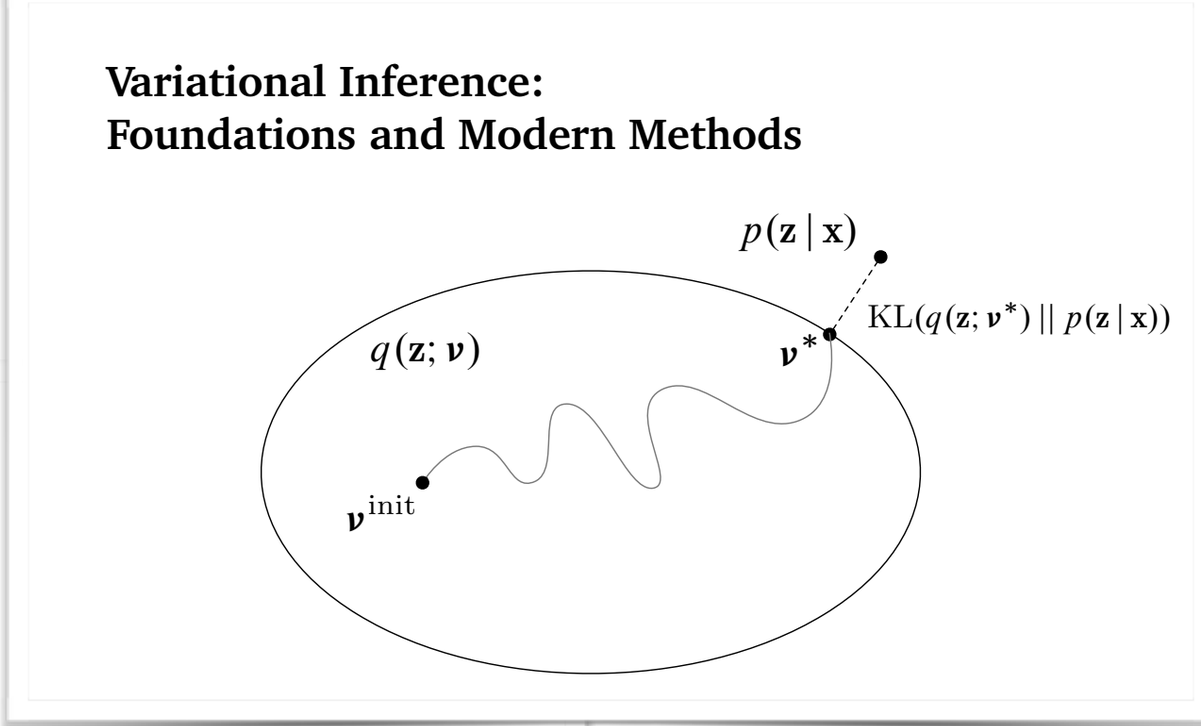
However, quality of inference will suffer if generative model isn't accurate



Celeste: Variational inference for a generative model of astronomical images

Regler, et al 33rd ICMLR, 2016

VARIATIONAL INFERENCE



The requirements for inference

The noisy gradient:

$$\frac{1}{S}\sum_{s=1}^{S} \nabla_{\nu} \log q(\mathbf{z}_s; \boldsymbol{\nu})(\log p(\mathbf{x}, \mathbf{z}_s) - \log q(\mathbf{z}_s; \boldsymbol{\nu})),$$

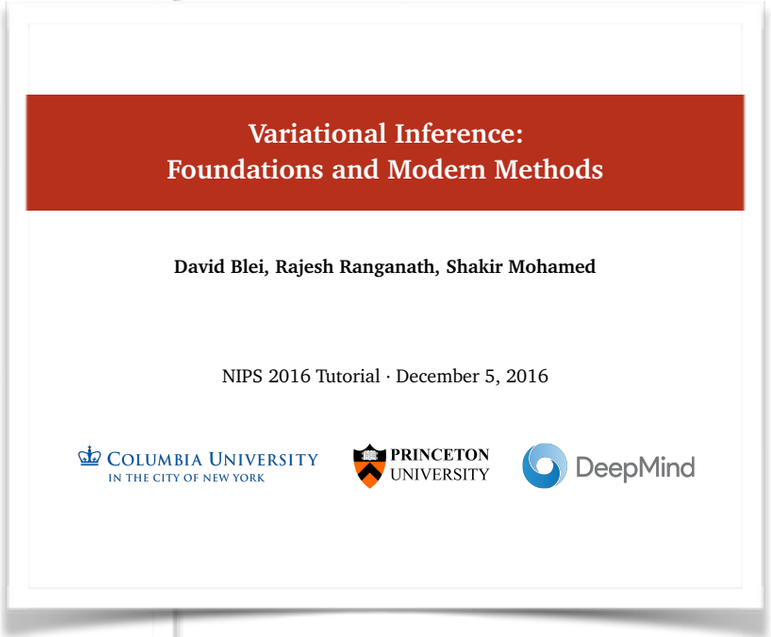
where $\mathbf{z}_s \sim q(\mathbf{z}; \boldsymbol{\nu})$

To compute the noisy gradient of the ELBO we need

- Sampling from $q(\mathbf{z})$
- Evaluating $\nabla_{\nu} \log q(\mathbf{z}; \boldsymbol{\nu})$
- Evaluating $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z})$

need likelihood for generative model

There is no model specific work: black box criteria are satisfied



VARIATIONAL AUTO-ENCODER

[Slides from D. Kingma NIPS 2015]

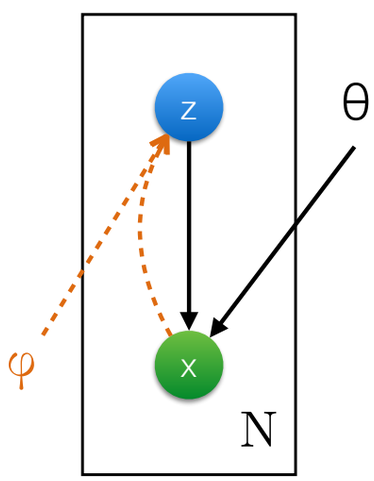
Learn a generative model for the data!

Diederik (Durk) Kingma

Max Welling

Auto-Encoding Variational Bayes

[Kingma and Welling, 2013/2014]
[Rezende et al, 2014]



- $q_\varphi(z|x) = N(\mu,\sigma^2)$
  $[\mu, \sigma^2] = f^{(z|x)}(x,\varphi) = \text{multilayer neural net}$
- Objective: lower bound of log p(x).
  - Jointly optimized w.r.t. φ and θ
  - This is approx. maximum likelihood
  - Simple SGD:
    - Sampling small minibatches of data
    - Sampling from approx. posterior
- This also minimizes an expected KL divergence
  $D_{KL}(q_\varphi(z|x)||p(z|x))$
  -> gives us cheap approx. inference for new datapoints

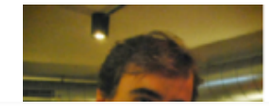
Kingma and Welling, Auto-encoding Variational Bayes, ICLR 2014
Rezende, Mohamed and Wierstra, Stochastic back-propagation and variational inference in deep latent Gaussian models, ICML 2014

Conv. net as encoder/decoder, trained on faces

VARIATIONAL AUTO-ENCODER

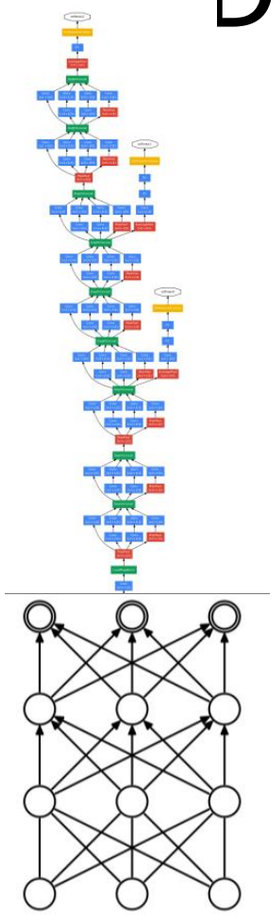
[Slides from D. Kingma NIPS 2015]

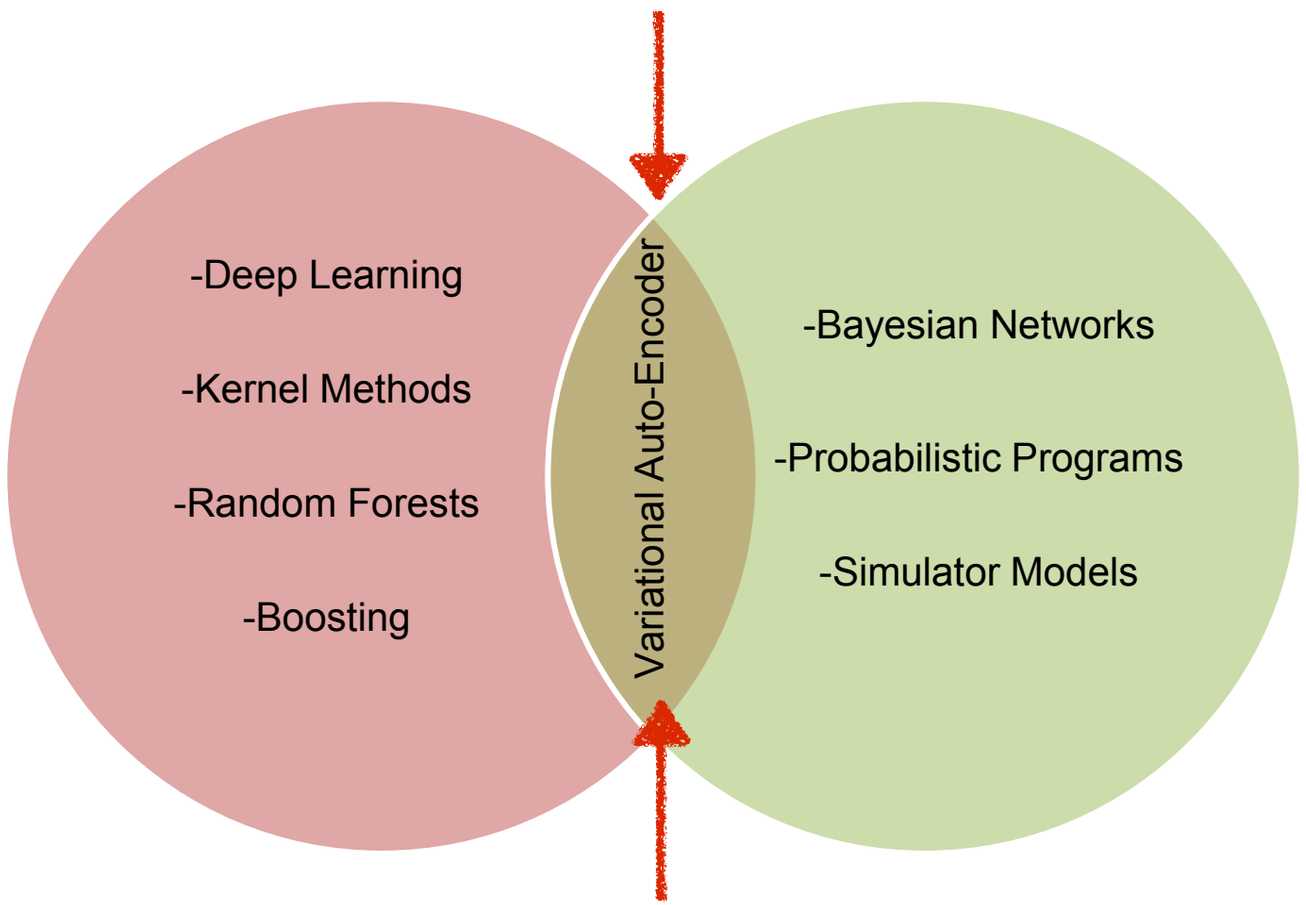
Learn a generative model for the data!

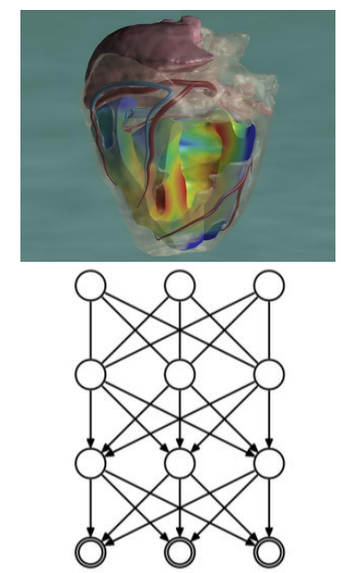


Max Welling

Discriminative or Generative?







- Advantages discriminative models:
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  - Efficient training algorithms available
  - Solve the problem you are evaluating on.
  - Very successful and accurate!
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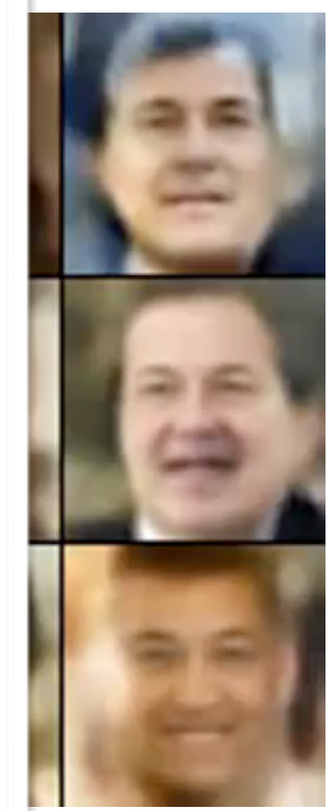


Edward

A library for probabilistic modeling, inference, and criticism.

Edward is a Python library for probabilistic modeling, inference, and criticism. It is a testbed for fast experimentation and research with probabilistic models, ranging from classical hierarchical models on small data sets to complex deep probabilistic models on large data sets. Edward fuses three fields: Bayesian statistics and machine learning, deep learning, and probabilistic programming.

It supports **modeling** with

Pyro

Pyro is a flexible, scalable deep probabilistic programming library built on PyTorch. Notably, it was designed with these principles in mind:

- **Universal**: Pyro is a universal PPL -- it can represent any computable probability distribution.
- **Scalable**: Pyro scales to large data sets with little overhead compared to hand-written code.
- **Minimal**: Pyro is agile and maintainable. It is implemented with a small core of powerful, composable abstractions.
- **Flexible**: Pyro aims for automation when you want it, control when you need it. This is accomplished through high-level abstractions to express generative and inference models, while allowing experts easy-access to customize inference.

LIKELIHOOD-FREE INFERENCE

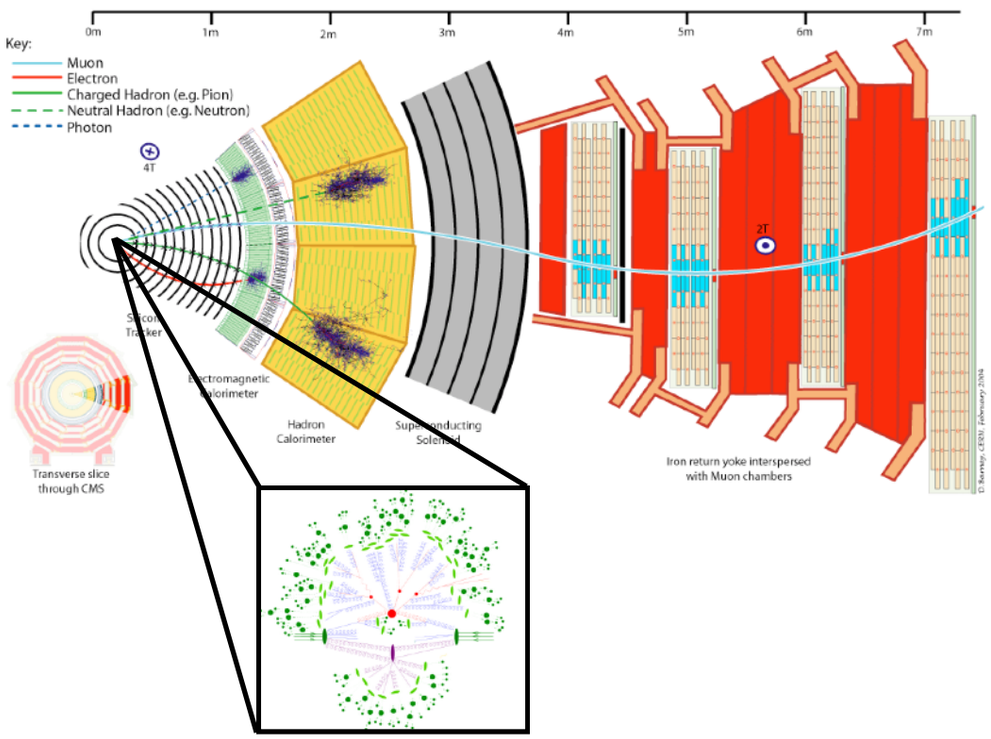
If you have a good generative model for the data and can evaluate likelihood, try variational inference… go for it!

But in many of our problems **we have a good simulation, but it's slow and likelihood is intractable**

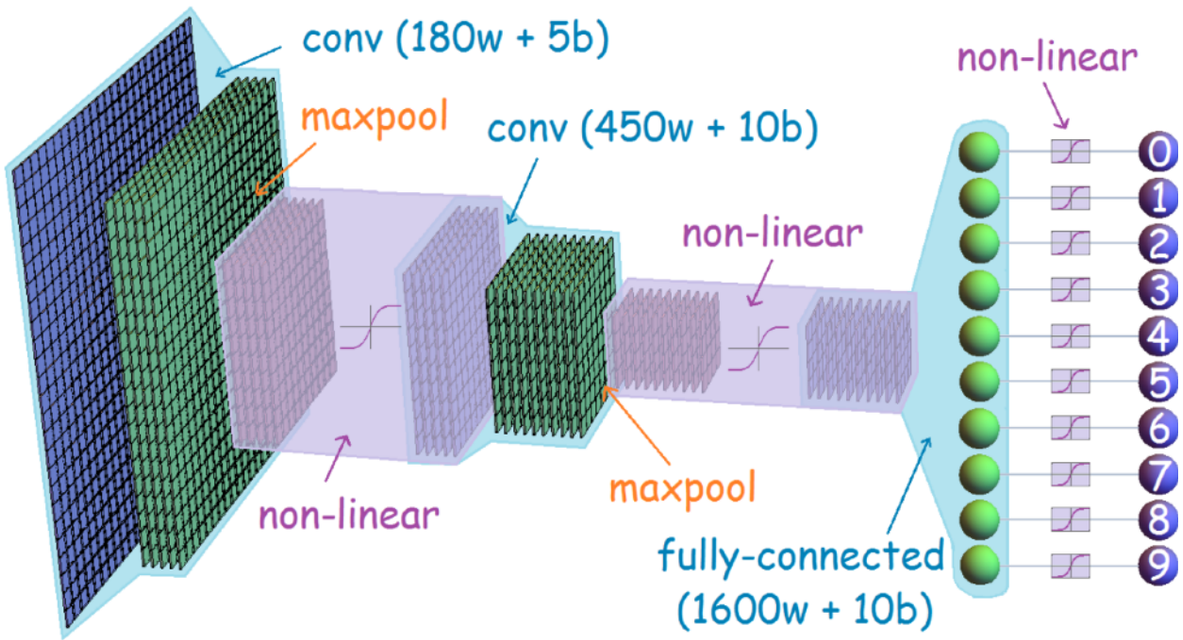
- Pythia/Sherpa
- GEANT
- GALPROP
- CORSIKA
- N-Body simulations
- gravitational lensing
- numerical GR for LIGO mergers

TWO APPROACHES TO LIKELIHOOD-FREE INFERENCE

Use simulator
(much more efficiently)



Learn simulator
(with deep learning)



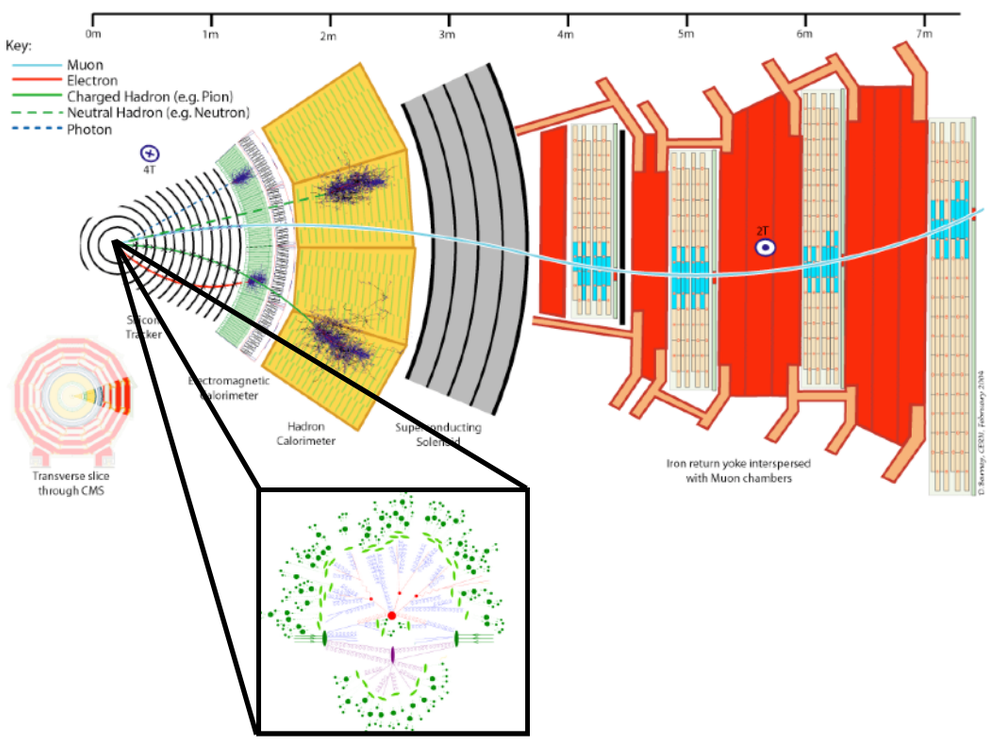
- Approximate Bayesian Computation (ABC)
- Probabilistic Programming
- Adversarial Variational Optimization (AVO)

- Generative Adversarial Networks (GANs), Variational Auto-Encoders (VAE)
- Likelihood ratio from classifiers (CARL)
- Autogregressive models, Normalizing Flows

[image credit: A.P. Goucher]

TWO APPROACHES

Use simulator
(much more efficiently)



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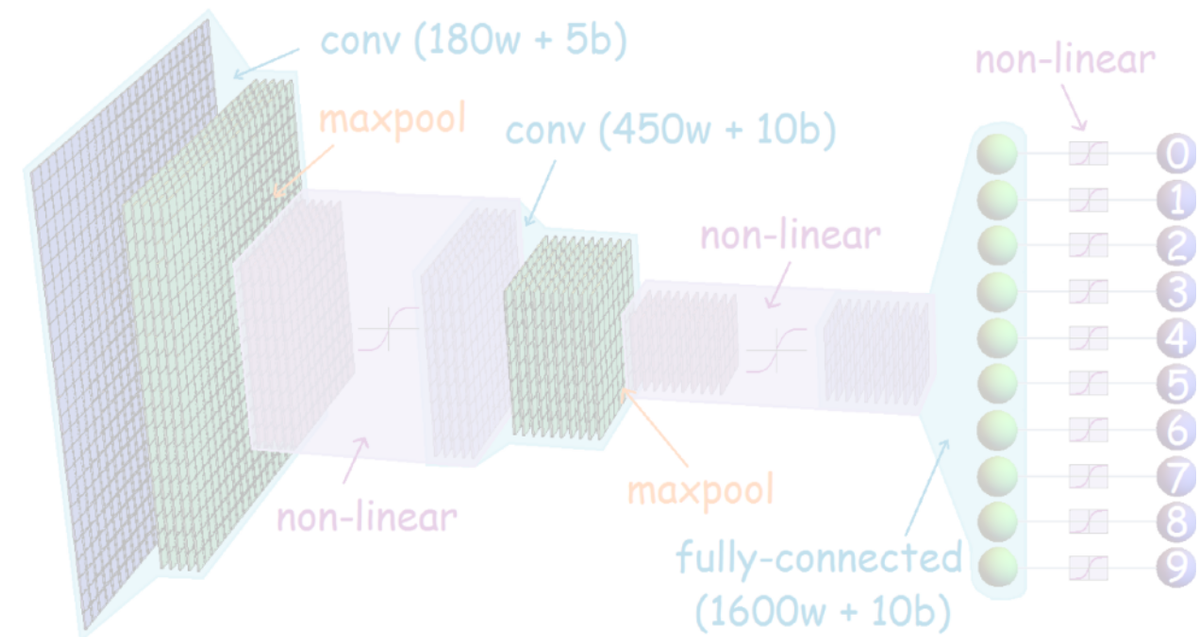

- Generative Adversarial Networks (GANs), Variational Auto-Encoders (VAE)
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- Autogregressive models, Normalizing Flows

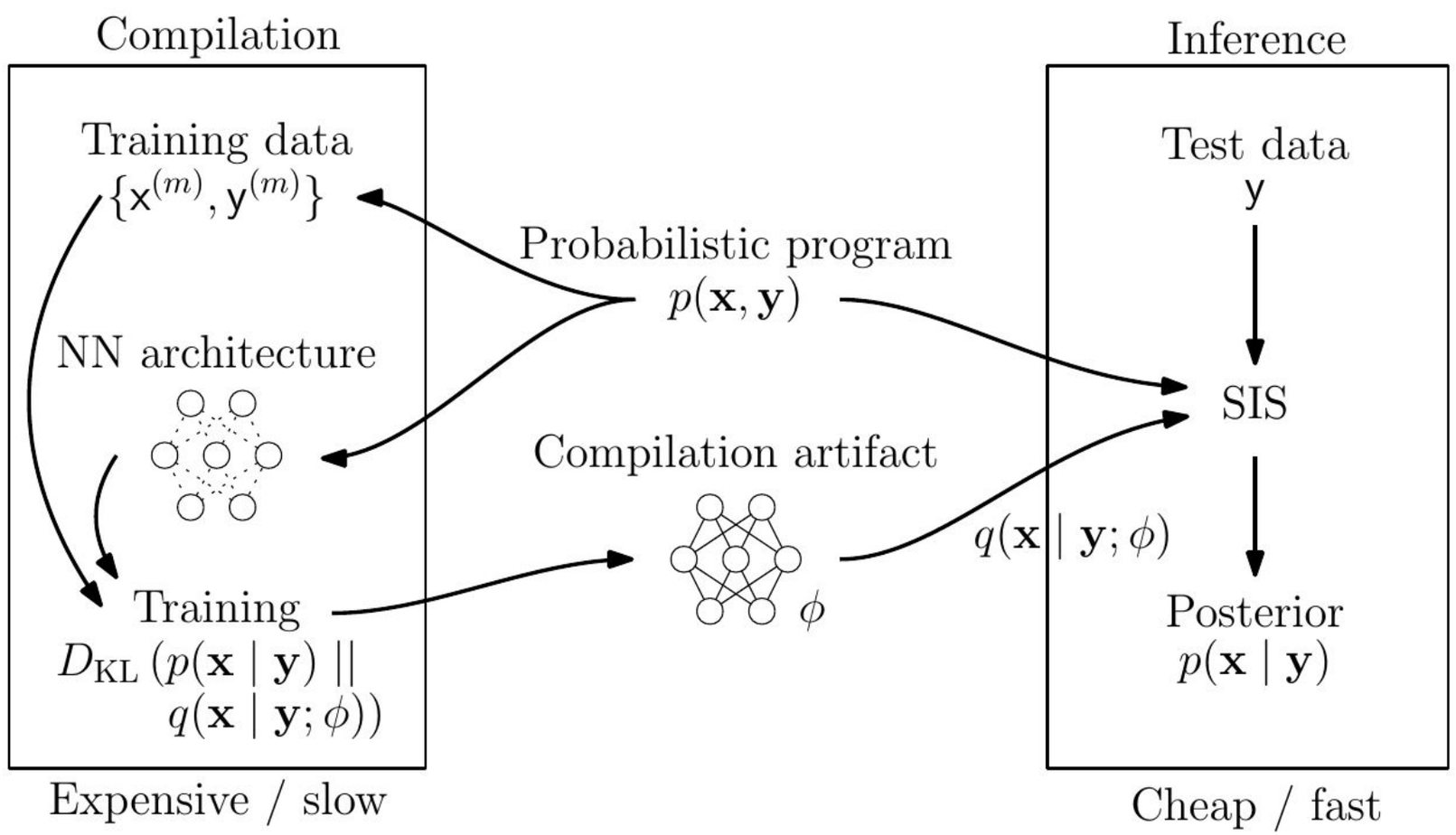
[image credit: A.P. Goucher]

HOW DOES IT WORK?

In short: hijack the random number generators and use NN's to perform a *very* smart type of importance sampling

Input: an inference problem denoted in a universal PPL (Anglican, CPProb)

Output: a trained inference network, or "compilation artifact" (Torch, PyTorch)



Le, Baydin and Wood. Inference Compilation and Universal Probabilistic Programming. AISTATS 2017. *arXiv:1610.09900*

IN PROGRESS: C++, SHERPA, GEANT4

Mario Lezcano Casado, Atılım Güneş Baydin, Tuan Anh Le, Frank Wood*
Department of Engineering Science
University of Oxford
{lezcano,gunes,tuananh,fwood}@robots.ox.ac.uk

Lukas Heinrich, Gilles Louppe, Kyle Cranmer
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New York University
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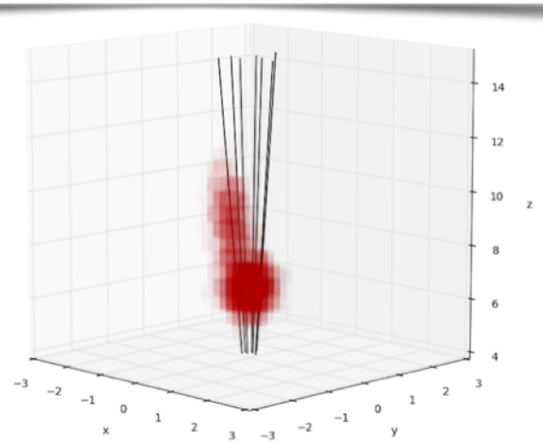
Wahid Bhimji, Prabhat
Lawrence Berkeley National Laboratory
{wbhimji,prabhat}@lbl.gov

Karen Ng
Intel
karen.y.ng@intel.com



Probabilistic programming with C++

Our new tool: CPProb
https://github.com/probprog/cpprob

Instrumenting C++ code to allow tools like SHERPA and GEANT run with inference compilation

```
void linear_regression(const std::array<std::pair<RealType, RealType>, N> & points) {
    using boost::random::normal_distribution;

    auto normal = normal_distribution<RealType>{0, 10};
    const auto a = cpprob::sample(normal, true);
    const auto b = cpprob::sample(normal, true);

    for (const auto & point : points) {
        auto likelihood = normal_distribution<RealType>{a * point.first + b, 1};
        cpprob::observe(likelihood, point.second);
    }
    cpprob::predict(a);
    cpprob::predict(b);
}
```

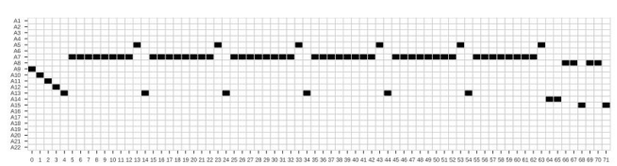
```
SHERPA::Hadron_Decays::Treat(ATOOLS::Blob_List*, double&)+0x709
SHERPA::Event_Handler::IterateEventPhases(SHERPA::eventtype::code&, double&)+0x1b2
SHERPA::Event_Handler::GenerateHadronDecayEvent(SHERPA::eventtype::code&)+0x979
```

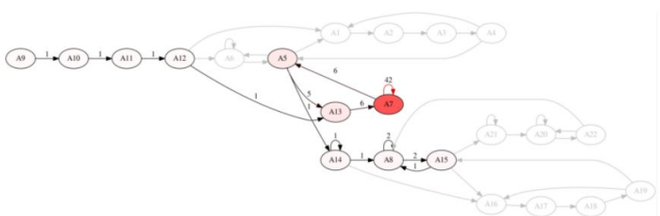
A case study in SHERPA & GEANT

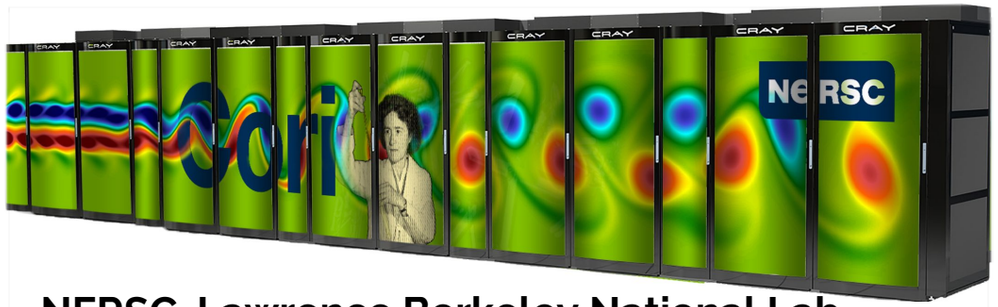
Probabilistic program analytics
allows us to **pinpoint "interesting" addresses** in execution traces
and corresponding **C++ code within SHERPA**

4.4.24 Unique trace T24

Length 72







NERSC, Lawrence Berkeley National Lab

Our current tools:
- CPProb
  - A new C++ PPL coupled with large-scale simulations using, e.g., SHERPA and GEANT
- PyTorch inference compilation backend
  - Dynamic computation graphs for NN artifacts

Designed to run on Cori at NERSC using Shifter

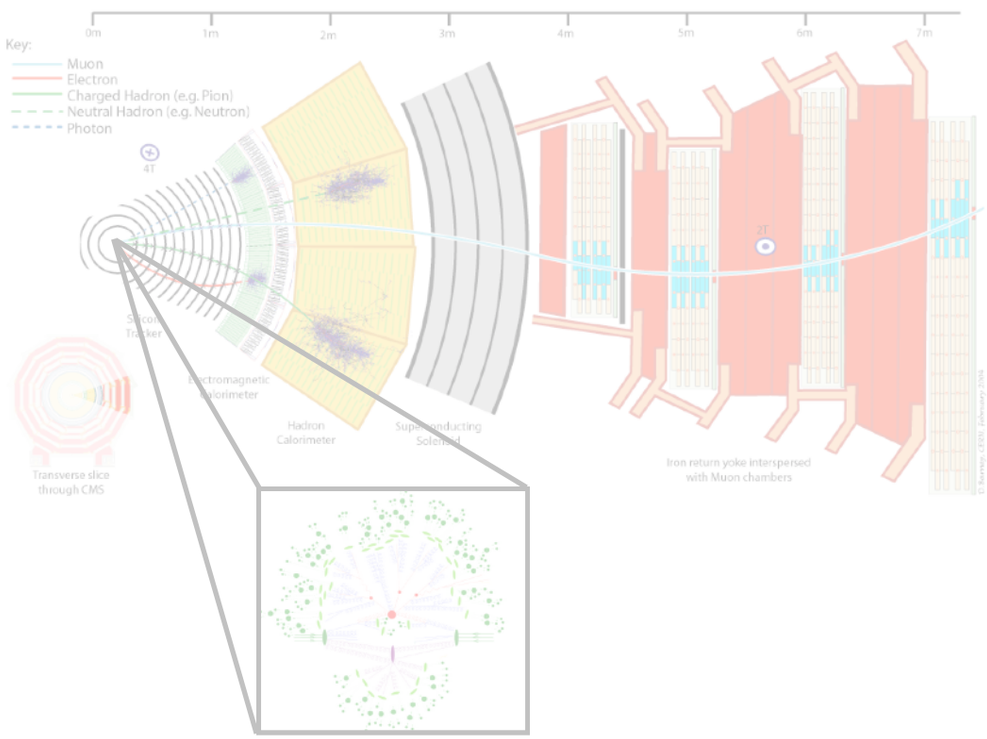
```
shifterimg -v pull docker:gbaydin/pytorch-infcomp:latest
shifterimg -v pull docker:gbaydin/sherpa-infcomp-full:latest
```

Slides from Atılım Güneş Baydin @ Hammers & Nails

https://dl4physicalsciences.github.io/files/nips_dlps_2017_30.pdf

TWO APPROACHES

Use simulator
(much more efficiently)



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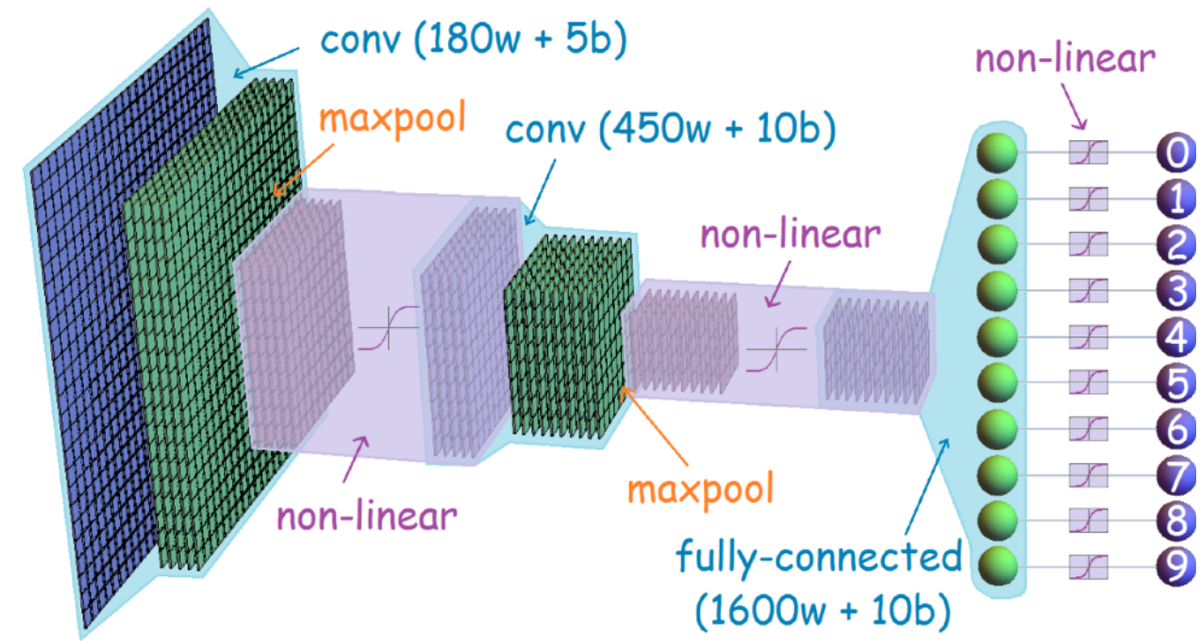

- Generative Adversarial Networks (GANs), Variational Auto-Encoders (VAE)
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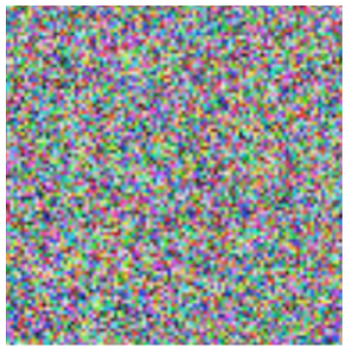
[image credit: A.P. Goucher]

LEARNING THE GENERATIVE MODEL

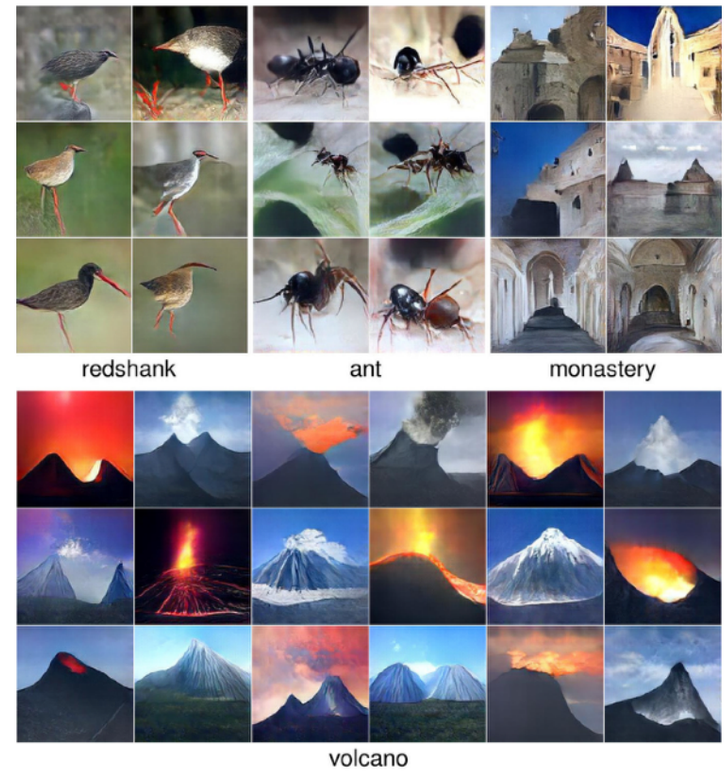
Z

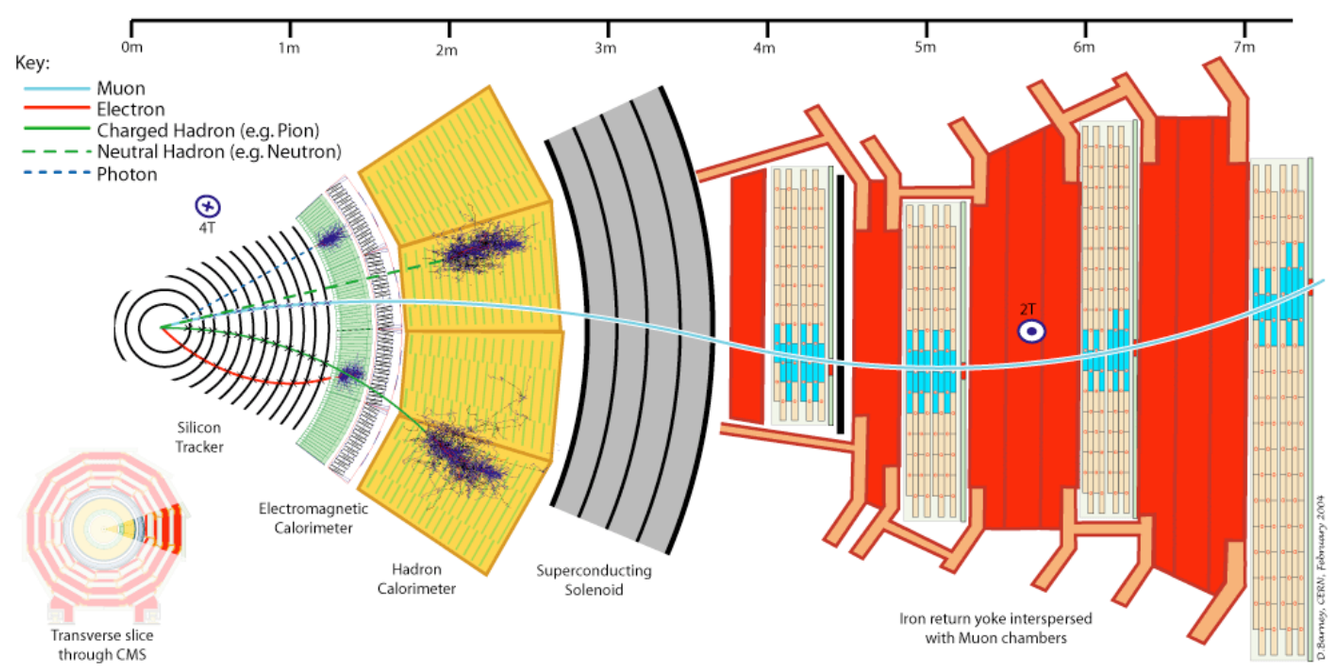
X

Noise ~ N(0,1)



Generative Model





http://torch.ch/blog/2015/11/13/gan.html

GANs FOR PHYSICS

CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks

Michela Paganini[a,b], **Luke de Oliveira**[a], **and Benjamin Nachman**[a]

[a] *Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA, 94720, USA*
[b] *Department of Physics, Yale University, New Haven, CT 06520, USA*

E-mail: michela.paganini@yale.edu, lukedeoliveira@lbl.gov, bnachman@cern.ch

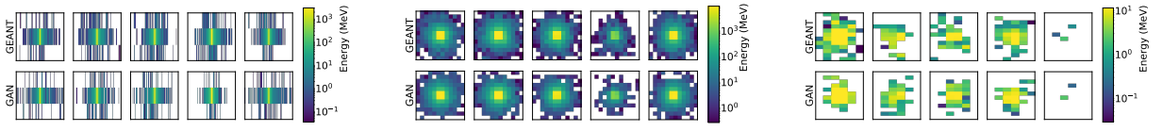


Figure 9: Five randomly selected e^+ showers per calorimeter layer from the training set (top) and the five nearest neighbors (by euclidean distance) from a set of CaloGAN candidates.

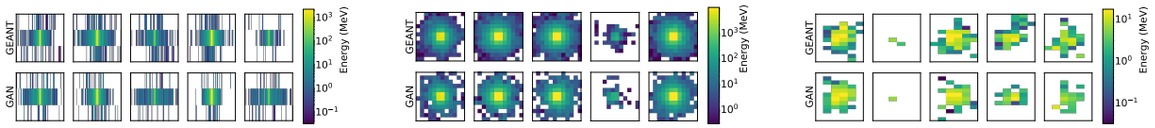


Figure 10: Five randomly selected γ showers per calorimeter layer from the training set (top) and the five nearest neighbors (by euclidean distance) from a set of CaloGAN candidates.

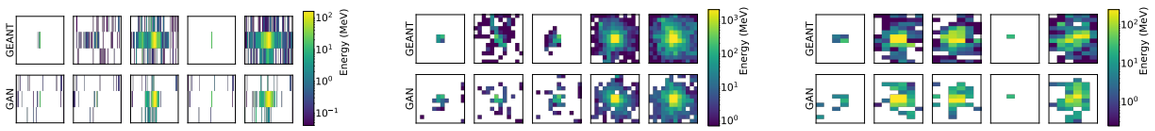
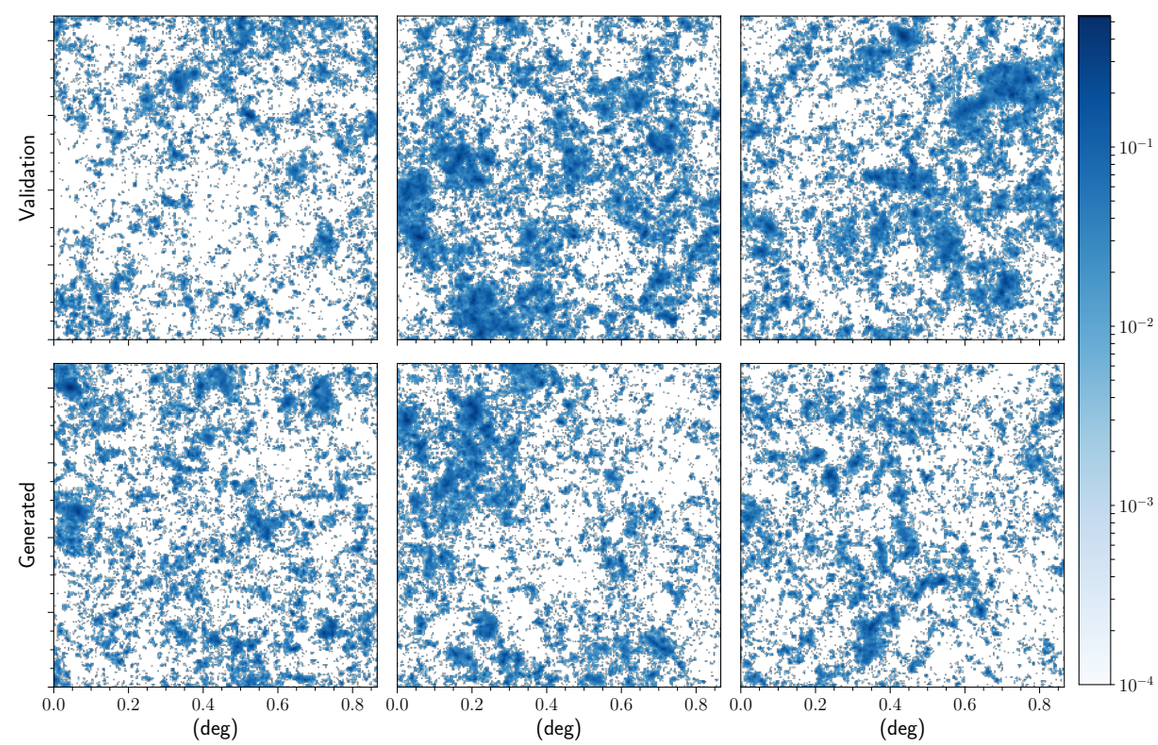


Figure 11: Five randomly selected π^+ showers per calorimeter layer from the training set (top) and the five nearest neighbors (by euclidean distance) from a set of CaloGAN candidates.

Creating Virtual Universes Using Generative Adversarial Networks

Mustafa Mustafa*[1], Deborah Bard[1], Wahid Bhimji[1], Rami Al-Rfou[2], and Zarija Lukić[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA 94720
[2]Google Research, Mountain View, CA 94043



WHY? GENERATIVE MODELS FOR CALIBRATION

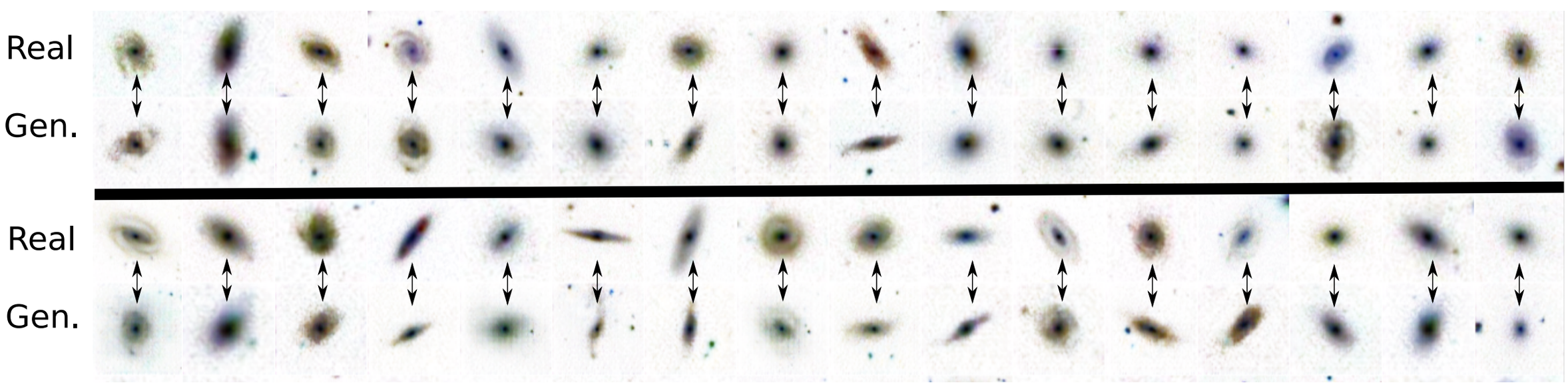
Use of generative models of galaxy images to help calibrate down-stream analysis in next-generation surveys.

Enabling Dark Energy Science with Deep Generative Models of Galaxy Images

Siamak Ravanbakhsh[1], François Lanusse[2], Rachel Mandelbaum[2], Jeff Schneider[1], and Barnabás Póczos[1]

[1]*School of Computer Science, Carnegie Mellon University*
[2]*McWilliams Center for Cosmology, Carnegie Mellon University*

***Abstract*—Understanding the nature of dark energy, the mysterious force driving the accelerated expansion of the Universe, is a major challenge of modern cosmology. The next generation of cosmological surveys, specifically designed to address this issue, rely on accurate measurements of the apparent shapes of distant galaxies. However, shape measurement methods suffer from various unavoidable biases and therefore will rely on a precise calibration to meet the accuracy requirements of the science analysis. This calibration process remains an open challenge as it requires large sets of high quality galaxy images. To this end, we study the application of deep conditional generative models in generating realistic galaxy images. In particular we consider variations on conditional variational autoencoder and introduce a new adversarial objective for training of conditional generative networks. Our results suggest a reliable alternative to the acquisition of expensive high quality observations for generating the calibration data needed by the next generation of cosmological surveys.**



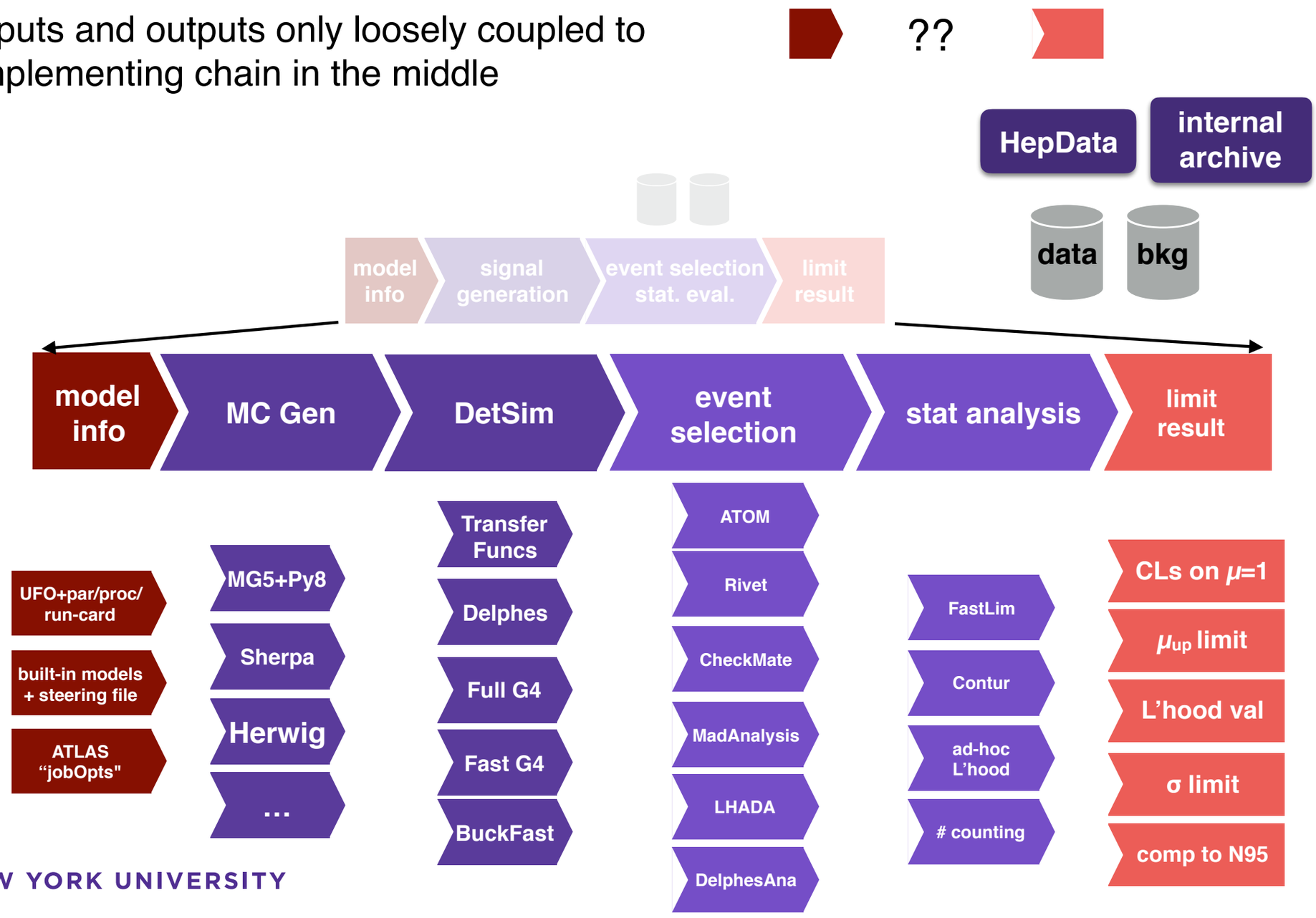
Accelerating and Improving

(Re)Interpretation

The Recipe for Reinterpretation

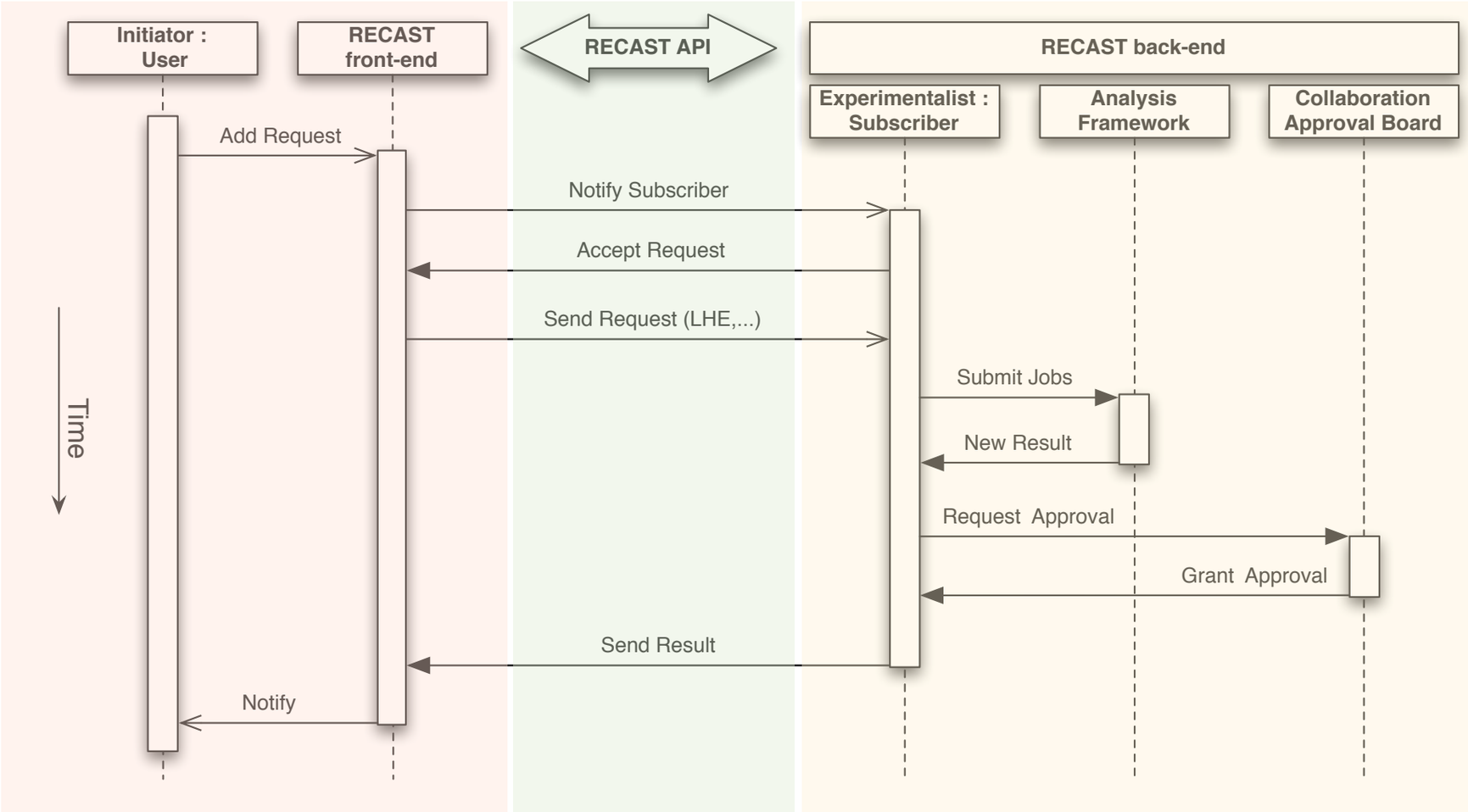
the recipe is the same for everyone — theorists and experimentalists

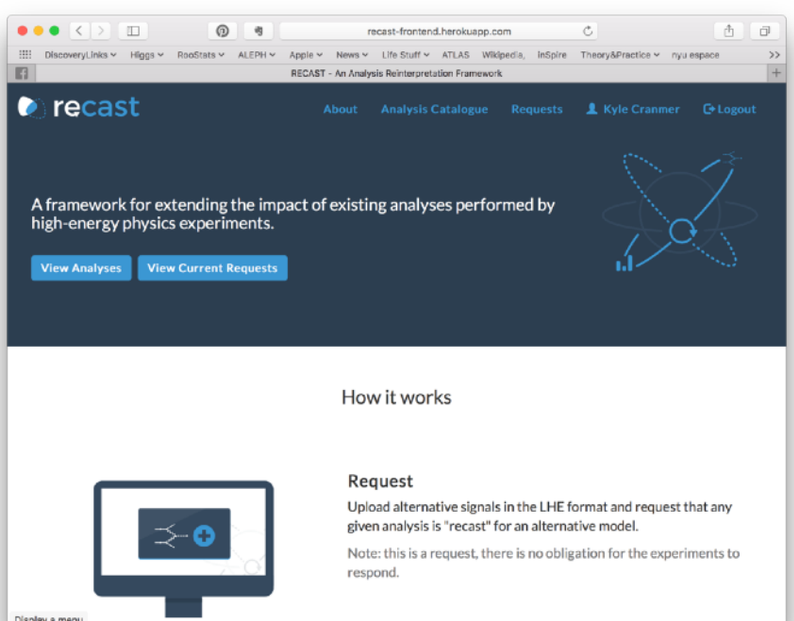
- inputs and outputs only loosely coupled to implementing chain in the middle



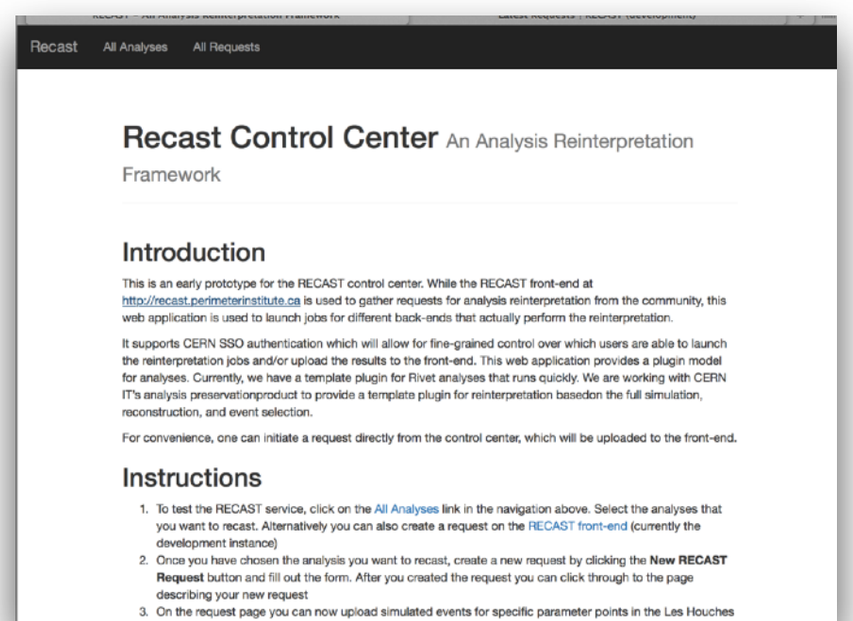
NEW YORK UNIVERSITY

slide from Lukas Heinrich

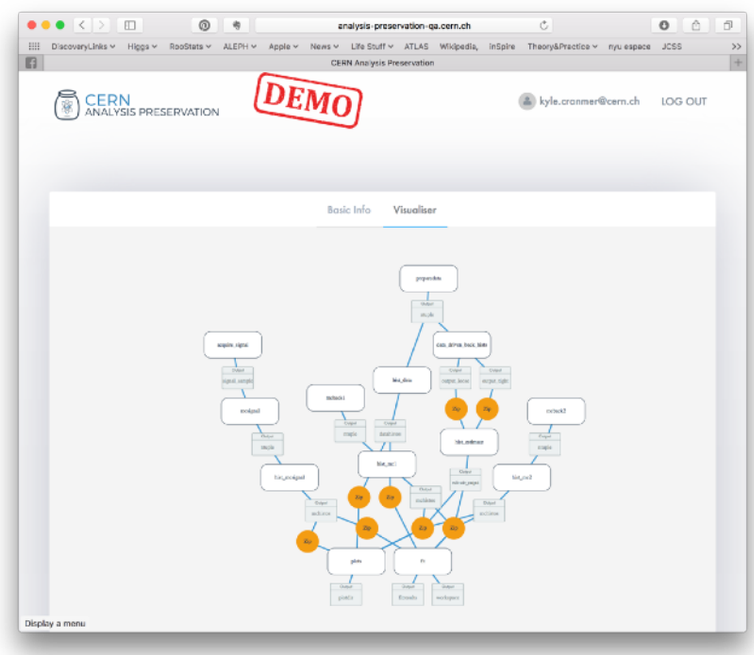




Front-End: public facing
collects requests



Control Center: not public, uses CERN auth.,
oversees processing of jobs on back-end



CERN Analysis Preservation:
Stores workflows, provides back-end
computing resources

SCIENTIFIC WORKLOWS IN THE CLOUD

Yadage and Packtivity – analysis preservation using parametrized workflows

Kyle Cranmer[1] **and Lukas Heinrich**[1]

[1] Department of Physics, New York University, New York, USA

E-mail: `lukas.heinrich@cern.ch`

Abstract. Preserving data analyses produced by the collaborations at LHC in a parametrized fashion is crucial in order to maintain reproducibility and re-usability. We argue for a declarative description in terms of individual processing steps – "packtivities" – linked through a dynamic directed acyclic graph (DAG) and present an initial set of JSON schemas for such a description and an implementation – "yadage" – capable of executing workflows of analysis preserved via Linux containers.

GitHub, Inc.

yadage - yaml based adage

DOI 10.5281/zenodo.309288 | pypi package 0.10.8 | build passing | health 94% | coverage 90% | docs latest | version git-master

A declarative way to define adage workflows using a JSON schema (but we'll always write it as YAML)

```
docker run --rm -it -v /var/run/docker.sock:/var/run/docker.sock -v $PWD:$PWD -w $PWD lukasheinrich/yada
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

or just

```
eval "$(curl https://raw.githubusercontent.com/diana-hep/yadage/master/yadagedocker.sh)"
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

This package reads and executes workflows adhering to the workflow JSON schemas defined at https://github.com/diana-hep/cap-schemas such as the onces stored in the community repository https://github.com/lukasheinrich/yadage-workflows. For executing the individual steps it mainly uses the packtivity python bindings provided by https://github.com/diana-hep/packtivity.

Possible Backends:

Yadage can run on various backends such as multiprocessing pools, ipython clusters, or celery clusters. If human intervention is needed for certain steps, it can also be run interactively.

Example Workflow

```
stages:
  - name: hello_world
```

reana.readthedocs.io

Fork me on GitHub

REANA - Reusable Analyses

build passing | coverage 100% | docs latest | Issues ready for work 2 | gitter join chat | license GNU General Public License v2.0

REANA is a system that permits to instantiate research data analyses on the cloud. It uses container-based technologies and was born to target the use case of particle physics analyses in LHC collaborations. The system paves the way to reusing and reinterpreting preserved data analyses even several years after the original analysis.

REANA - Reusable Analyses

Navigation

REANA@DockerHub
REANA@GitHub

Quick search

Go

v: latest

https://arxiv.org/pdf/1706.01878.pdf

RECASTING THROUGH REWEIGHTING

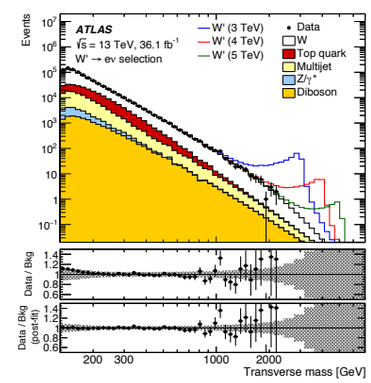
We can accelerate recasting via reweighting

$$p_1(x) = \int p_1(z) W(x|z) dz = \int p_0(z) \underbrace{\frac{p_1(z)}{p_0(z)}}_{\text{reweighting}} W(x|z) dz$$

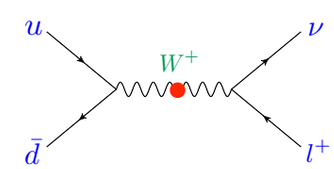
- Simulated events provide (truth, reco) pairs (z_i, x_i)
- reweight events ratio of BSM/SM cross-section at truth level
- **pros**: fast! still able to advantages of folding approach
- **cons**: need some book-keeping to know z_i and $p_0(z_i)$. Weights should be ~1 (ok for EFT, not for very different topology)

18

3) reweight folded samples



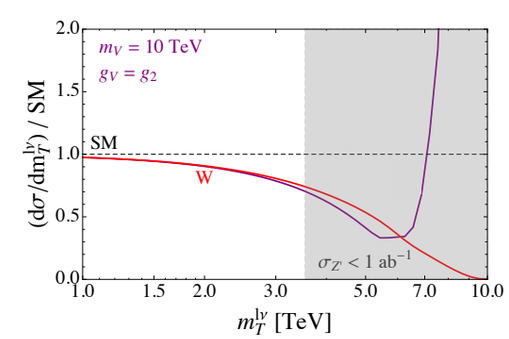
repurpose W' search for EFT bounds?



$$\frac{1}{\Lambda_W^2}(D_\rho W^a_{\mu\nu})^2$$

- reweight events by truth σ:

$$w_i = \frac{\sigma_{\Lambda_W}}{\sigma_{SM}}(m_T^i)$$



- Cranmer, Farina, Heinrich, Pappadopulo, JTR, *to appear*

http://beta.briefideas.org/ideas/8106c030eba22dd3a8d268940d5e42d8

HIGH DIMENSIONAL REWEIGHTING

$$p_1(x) = \int p_1(z) W(x|z) dz = \int p_0(z) \underbrace{\frac{p_1(z)}{p_0(z)}}_{\text{reweighting}} W(x|z) dz$$

In order to reweight events, we need to be able to evaluate $p_1(z)/p_0(z)$. There are a few options:

- we simply estimate $p_1(z)$ & $p_0(z)$ from generated samples with histograms (works if z is 1- or 2- dimensional)
- we have access to differential cross-section code that we can evaluate ratio for any z [eg. MadWeight, MadMax, PDF uncertainties, …]
- But what if we have samples of high-dimensional z and don't have an effective way to evaluate $p_1(z)$ & $p_0(z)$?

CARL

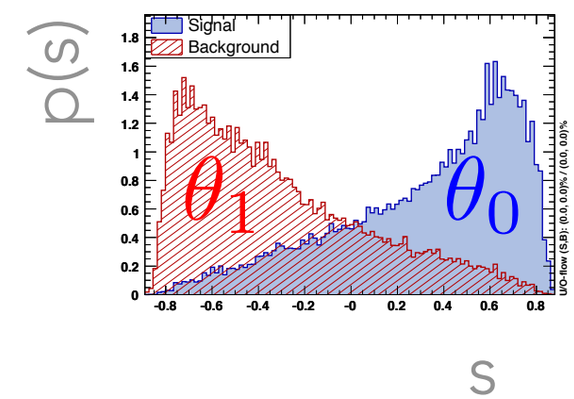
notation: here I use x, but could be z

The intractable likelihood ratio based on high-dimensional features x is:

$$\frac{p(x|\theta_0)}{p(x|\theta_1)}$$

We can show that an **equivalent test** can be made from 1-D projection

$$\frac{p(x|\theta_0)}{p(x|\theta_1)} = \frac{p(s(x;\theta_0,\theta_1)|\theta_0)}{p(s(x;\theta_0,\theta_1)|\theta_1)}$$



if the scalar map s: X → $\mathbb{R}$ has the same level sets as the likelihood ratio

$$s(x;\theta_0;\theta_1) = \text{monotonic}[\ p(x|\theta_0)/p(x|\theta_1)\ ]$$

Estimating the density of $s(x;\theta_0,\theta_1)$ via the simulator calibrates the ratio.

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

Binary classifier on balanced y=0 and y=1 labels learns

$$s(x) = \frac{p(x|y=1)}{p(x|y=0) + p(x|y=1)}$$

Which is one-to-one with the likelihood ratio

$$\frac{p(x|y=0)}{p(x|y=1)} = 1 - \frac{1}{s(x)}$$

Can do the same thing for any two points θ_0 & θ_1 in parameter space. I call this a **parametrized classifier**

$$s(x;\theta_0,\theta_1) = \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}$$

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

CARL SOFTWARE

Gilles Louppe

http://diana-hep.org/carl/

diana-hep.org

DiscoveryLinks Higgs RooStats ALEPH Apple News Life Stuff ATLAS Wikipedia, inSpire Theory&Practice nyu espace JCSS HCG

Meet F | Jupyter Note... | Weekend rea... | early-career-... | 2016 Electio... | 12-day Event... | Joint meetin... | carl API

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Index

Sub-modules

- carl.data
- carl.distributions
- carl.learning
- carl.ratios

Notebooks

- Composing and fitting distributions
- Diagnostics for approximate likelihood ratios
- Likelihood ratios of mixtures of normals
- Parameterized inference from multidimensional data
- Parameterized inference with nuisance parameters

Display a menu

carl module

`carl` is a toolbox for likelihood-free inference in Python.

The likelihood function is the central object that summarizes the information from an experiment needed for inference of model parameters. It is key to many areas of science that report the results of classical hypothesis tests or confidence intervals using the (generalized or profile) likelihood ratio as a test statistic. At the same time, with the advance of computing technology, it has become increasingly common that a simulator (or generative model) is used to describe complex processes that tie parameters of an underlying theory and measurement apparatus to high-dimensional observations. However, directly evaluating the likelihood function in these cases is often impossible or is computationally impractical.

In this context, the goal of this package is to provide tools for the likelihood-free setup, including likelihood (or density) ratio estimation algorithms, along with helpers to carry out inference on top of these.

This project is still in its early stage of development. Join us on GitHub if you feel like contributing!

build passing | coverage 91% | DOI 10.5281/zenodo.47798

Likelihood-free inference with calibrated classifiers

Extensive details regarding likelihood-free inference with calibrated classifiers can be found in the companion paper *"Approximating Likelihood Ratios with Calibrated Discriminative Classifiers", Kyle Cranmer, Juan Pavez, Gilles Louppe.* http://arxiv.org/abs/1506.02169

Installation

The following dependencies are required:

- Numpy >= 1.11

LEARNING THE EXCLUSION SURFACE

There are a few groups that are using machine learning to learn the likelihood surface L(θ) - or equivalently CLs(θ) - for a particular new physics model with parameters θ

Some variants are estimating expected signal event counts s(θ) directly (to later plug into some simplified likelihood)

- **note**: this is restricted to a particular physics model
- **note**: some traditional recasting tool is still needed to produce training data

In this restricted setting, what else can we do?

LEARNING DEPENDENCE ON MODEL PARAMETERS

The BSM-AI project: SUSY-AI – generalizing LHC limits on supersymmetry with machine learning

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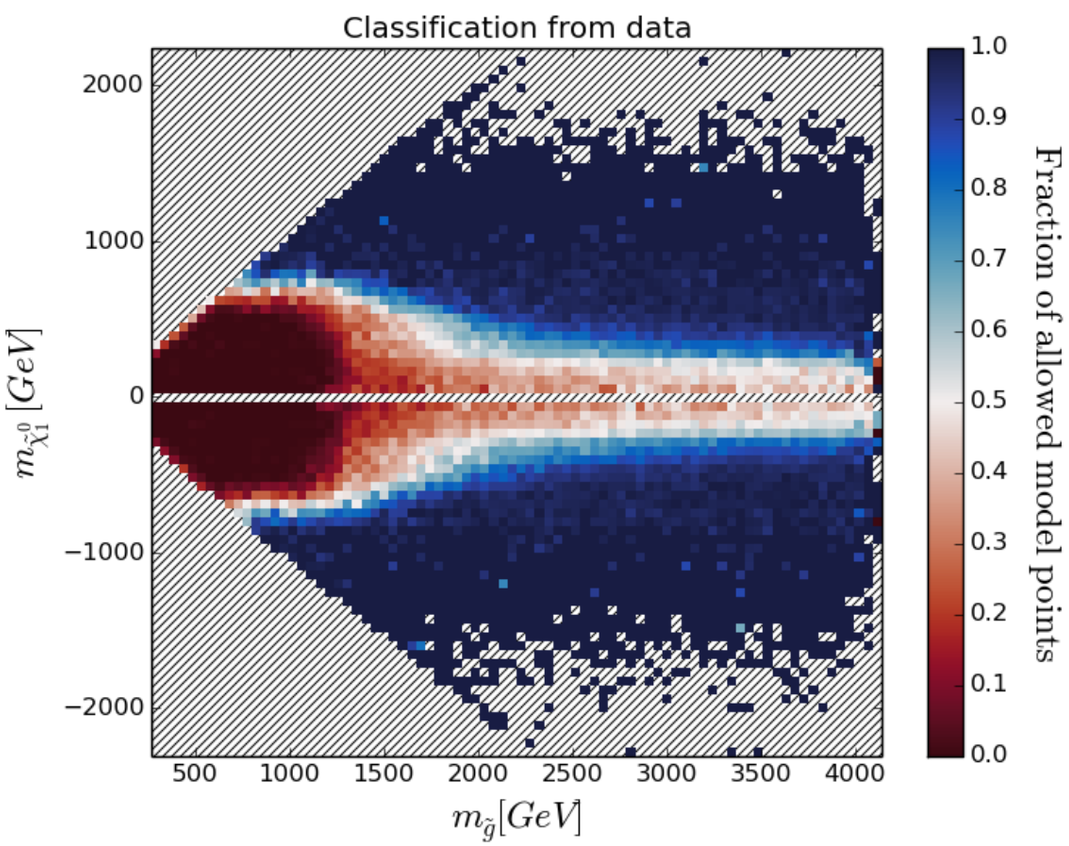

Accelerating the BSM interpretation of LHC data with machine learning

Gianfranco Bertone,[1] Marc Peter Deisenroth,[2] Jong Soo Kim,[3]
Sebastian Liem,[1] Roberto Ruiz de Austri,[4] and Max Welling[5]

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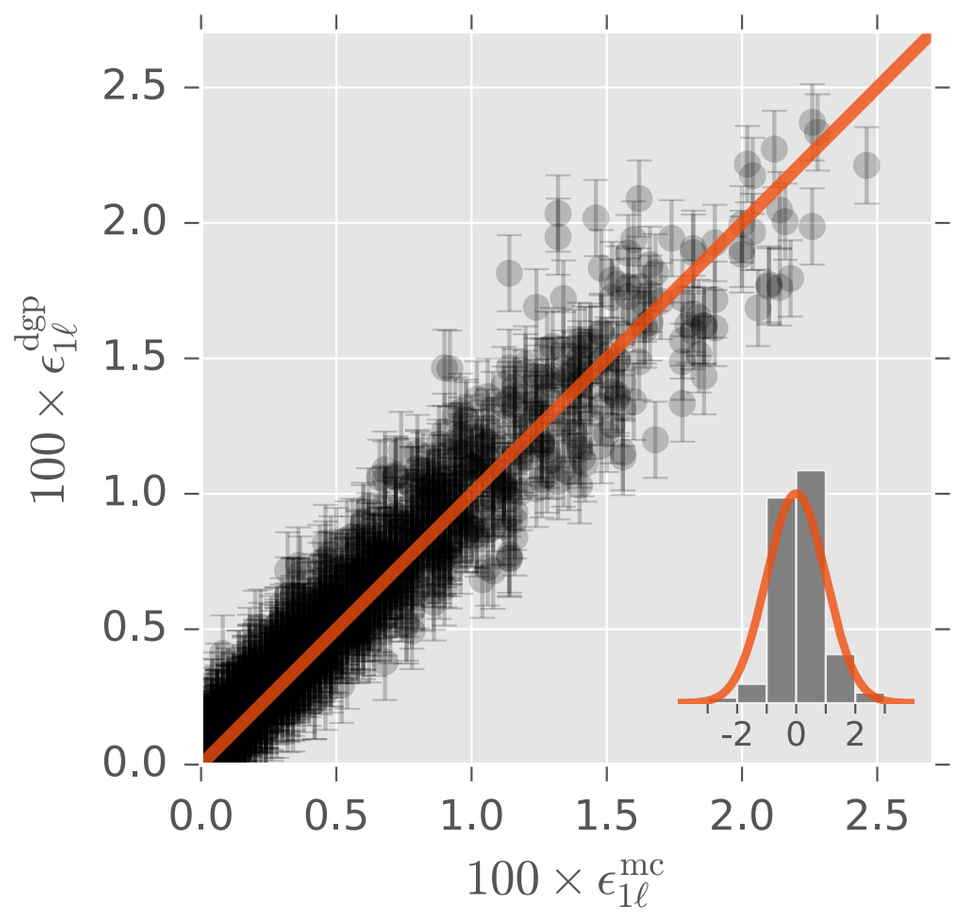
(Dated: November 10, 2016)

The interpretation of Large Hadron Collider (LHC) data in the framework of Beyond the Standard Model (BSM) theories is hampered by the need to run computationally expensive event generators and detector simulators. Performing statistically convergent scans of high-dimensional BSM theories is consequently challenging, and in practice unfeasible for very high-dimensional BSM theories. We present here a new machine learning method that accelerates the interpretation of LHC data, by learning the relationship between BSM theory parameters and data. As a proof-of-concept, we demonstrate that this technique accurately predicts natural SUSY signal events in two signal regions at the High Luminosity LHC, up to four orders of magnitude faster than standard techniques. The new approach makes it possible to rapidly and accurately reconstruct the theory parameters of complex BSM theories, should an excess in the data be discovered at the LHC.



INFORMATION GEOMETRY

If one can learn how number of events and distributions depend on parameters, then can utilize information geometry to characterize phenomenology & provide forecasts

Better Higgs Measurements Through Information Geometry

Johann Brehmer,[1] Kyle Cranmer,[2] Felix Kling,[3] and Tilman Plehn[1]

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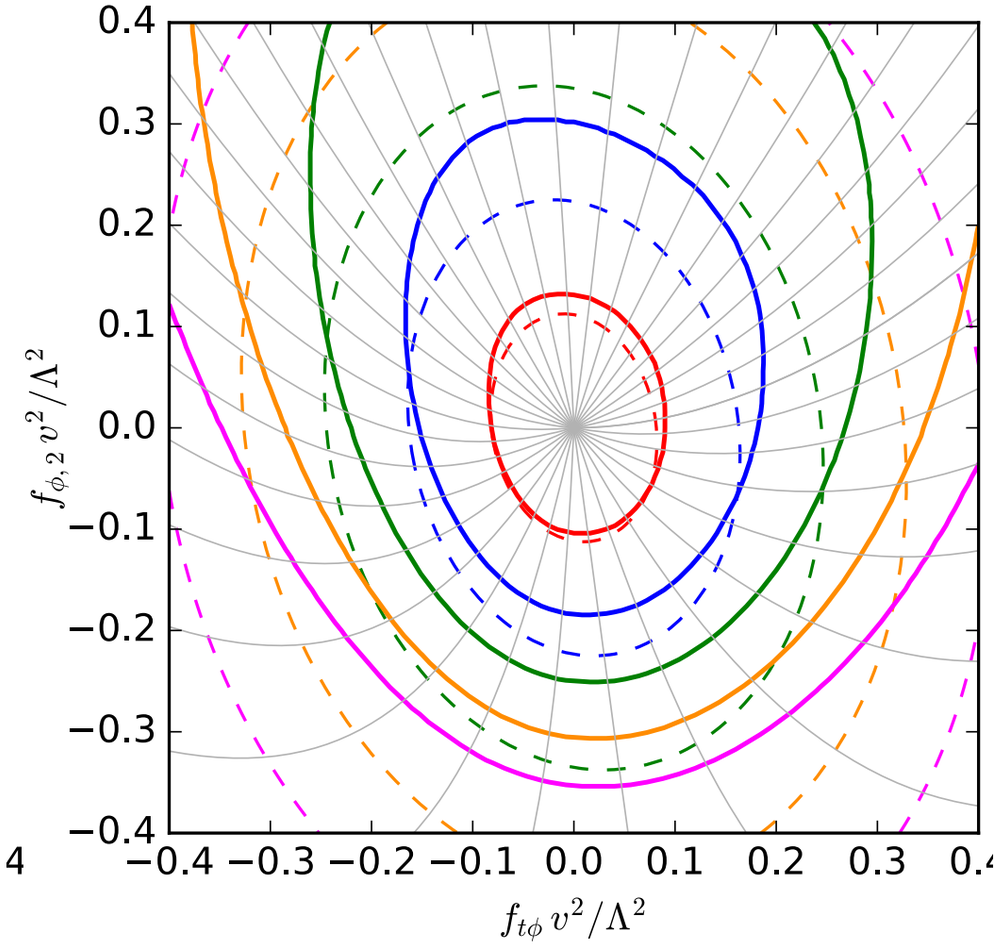
[2] *Center for Cosmology & Particle Physics, New York University, USA*
[3] *University of California, Irvine, USA*
(Dated: March 31, 2017)



A Fresh Approach to Forecasting in Astroparticle Physics and Dark Matter Searches

Thomas D. P. Edwards[1,*] and Christoph Weniger[1,†]

[1] *Gravitation Astroparticle Physics Amsterdam (GRAPPA),*
Institute for Theoretical Physics Amsterdam and Delta Institute for Theoretical Physics,
University of Amsterdam, Science Park 904, 1090 GL Amsterdam, The Netherlands
(Dated: Compiled on April 20, 2017)

swordfish: Efficient Forecasting of New Physics Searches without Monte Carlo

Thomas D. P. Edwards[1,*] and Christoph Weniger[1,†]

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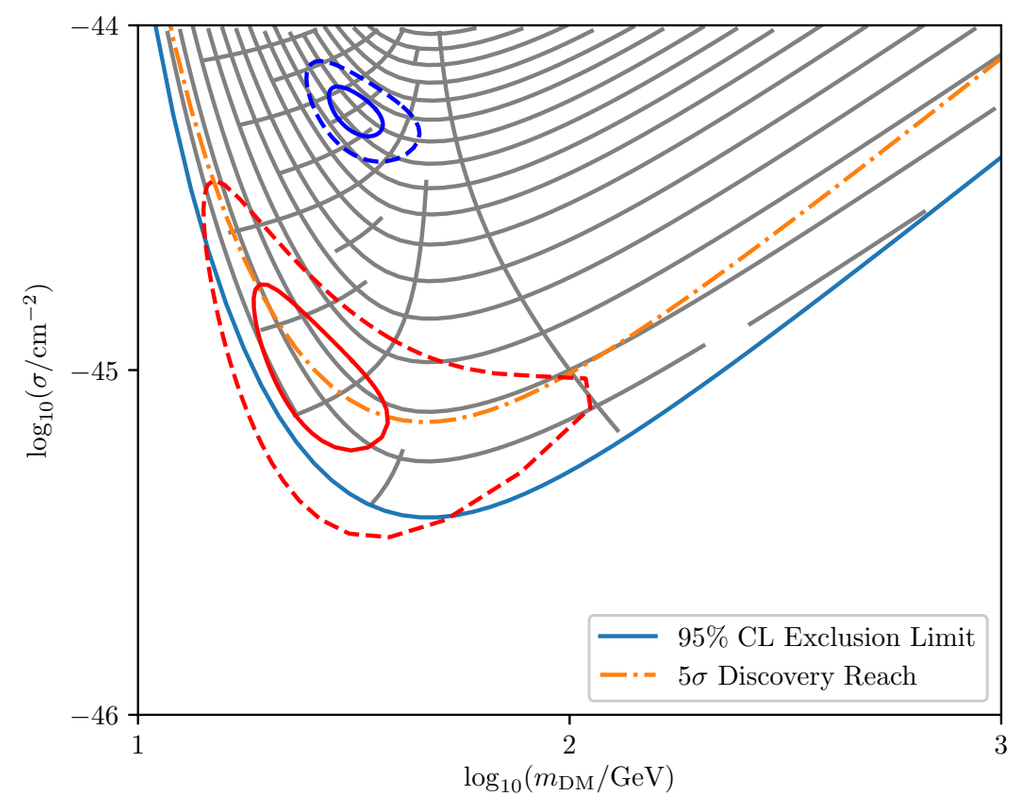
Institute for Theoretical Physics Amsterdam and Delta Institute for Theoretical Physics,
University of Amsterdam, Science Park 904, 1090 GL Amsterdam, The Netherlands
(Dated: Compiled on December 15, 2017)



INFORMATION GEOMETRY & NN'S

Brehmer, Cranmer, Kling, Plehn
https://arxiv.org/abs/1612.05261

If we have a binned analysis, then the total likelihood is

$$f(\mathbf{n}|\boldsymbol{\nu}) = \prod_c \mathrm{Pois}(n_c|\nu_c) = \prod_c \frac{\nu_c^{n_c} e^{-\nu_c}}{n_c!} \,.$$

where ν_c are expected signal+background for c^{th} bin.

Information geometry gives metric tensor over theory space and describes expected covariance matrix.

We can calculate the Fisher information in terms of the Poisson mean $\boldsymbol{\nu}$ as

$$\frac{\partial \log f}{\partial \nu_c} = \frac{n_c}{\nu_c} - 1 \qquad \frac{\partial^2 \log f}{\partial \nu_c \partial \nu_{c'}} = -\frac{\delta_{cc'}\, n_c}{\nu_c^2} \qquad I_{cc'} \equiv -E\left[\frac{\partial^2 \log f}{\partial \nu_c \partial \nu_{c'}}\middle|\boldsymbol{\nu}\right] = \frac{\delta_{cc'}}{\nu_c} \,. \tag{A2}$$

If we express the expected count rates in terms of model parameters g_i, the Fisher information becomes

$$I_{ij} = \sum_c \frac{1}{\nu_c} \frac{\partial \nu_c}{\partial g_i} \frac{\partial \nu_c}{\partial g_j} \,. \tag{A3}$$

The matrix $\partial \nu_c / \partial g_i$ is determined by selection requirements, detector acceptance, and efficiencies. In the κ framework that only scales cross sections and branching ratios, the matrix $\partial \nu_c / \partial g_i$ is trivial to calculate in closed form. For each channel this matrix is singular, which means it measures one direction in parameter space and is blind to all others. At least as many channels as parameters are required to make the combined information in Eq. (A3) non-singular and remove all blind directions (assuming the channels do not provide degenerate information, i. e. the same eigenvectors in the Fisher information).

If we learn $\nu(\theta)$ with a neural network, we can easily compute the Jacobian $\partial \nu / \partial \theta$!

We can use this to efficiently sample the parameter space!

want constant # samples per expected error ellipse

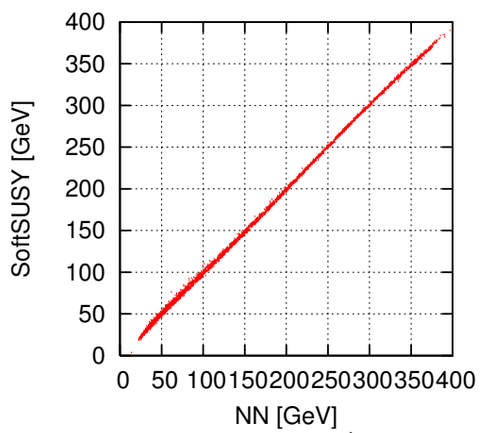
notation: $g=\theta$ are parameters of theory

LEARNING SPECTRUM CALCULATORS

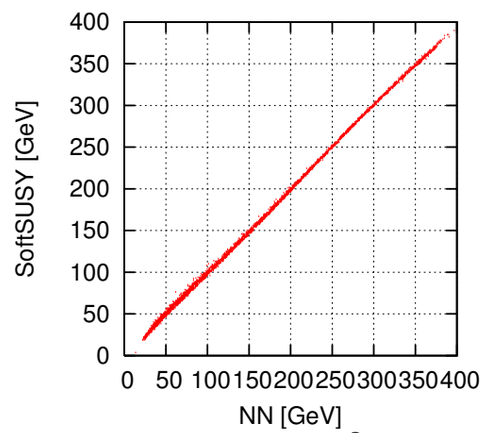
Bridges, Cranmer, Feroz, Hobson, Ruiz de Austri, Trotta, https://arxiv.org/abs/1011.4306

we can chain this process… eg. learn dependence of counts on physical masses, and then learn dependence of masses on theory parameters.

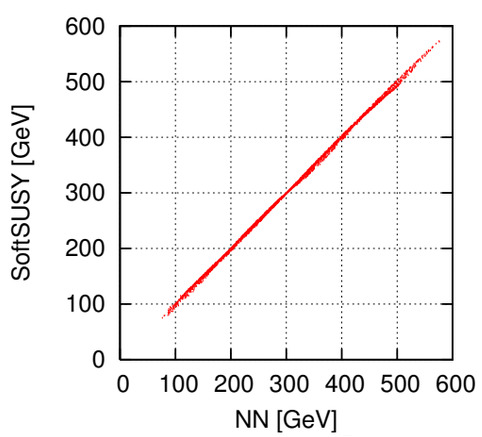
- if it's differentiable, we can calculate Jacobian and "pull back"



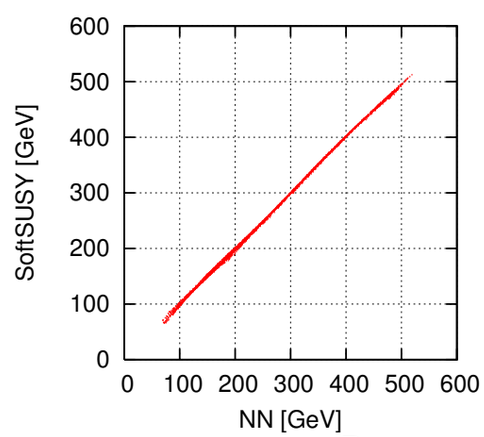
(a) m_ν^1



(b) m_ν^2

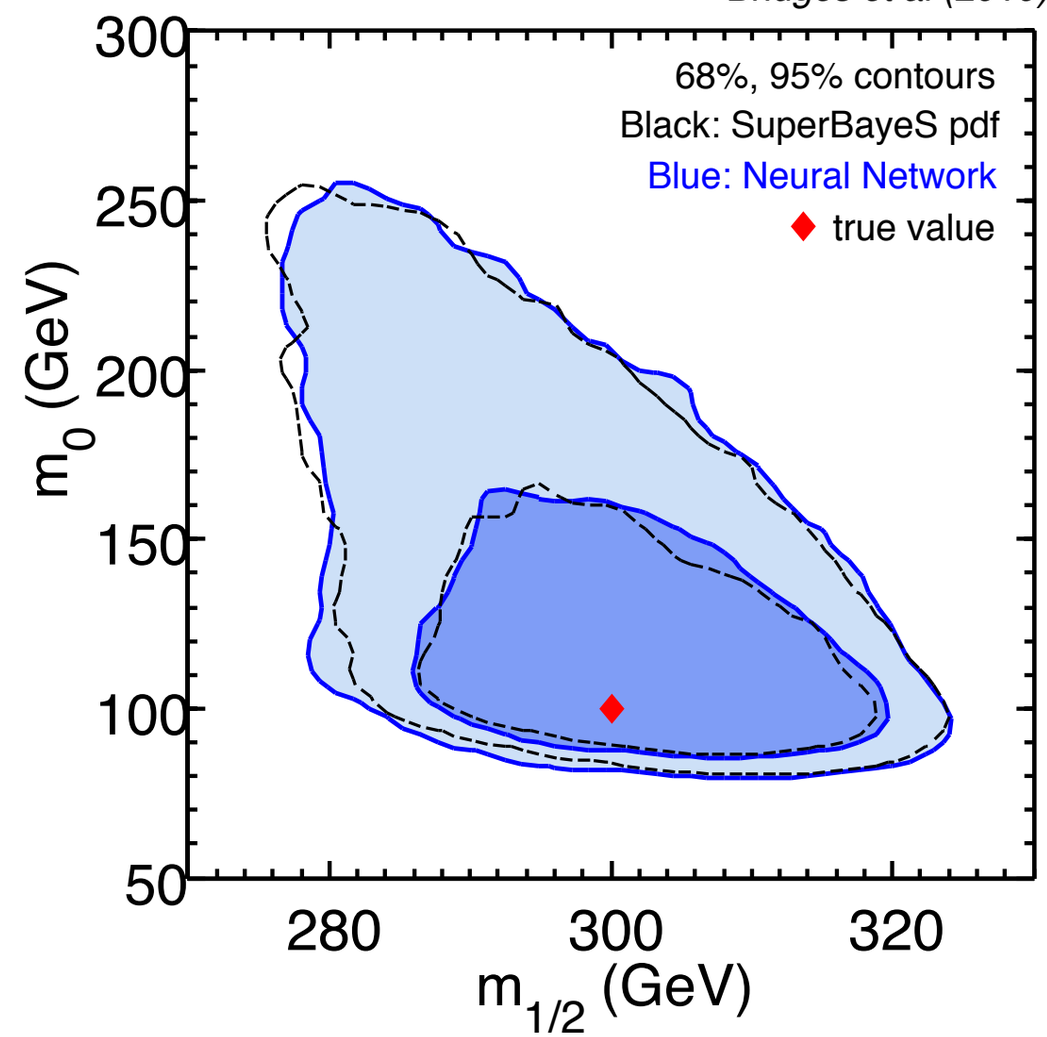


(d) m_{se}^L



(e) $m_{s\mu}^R$

Bridges et al (2010)

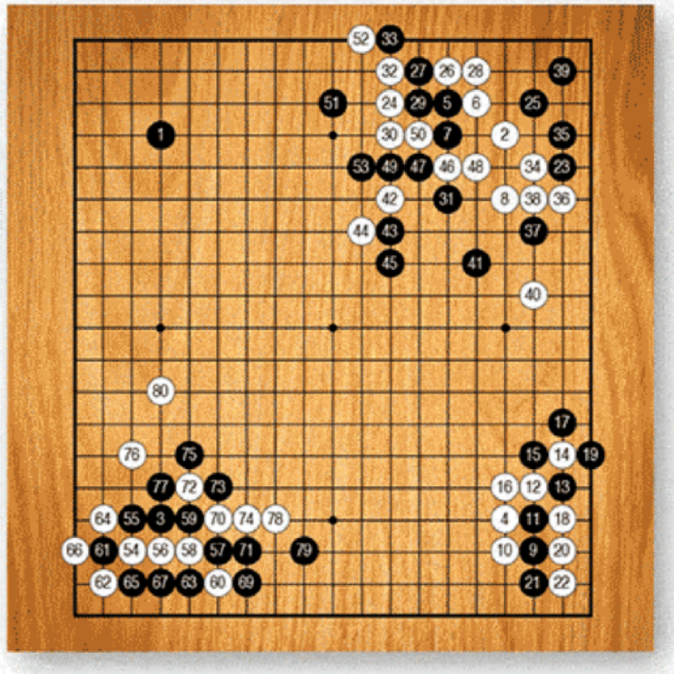


A Coverage Study of the CMSSM Based on ATLAS Sensitivity Using Fast Neural Networks Techniques

Decision Making
&
Reinforcement Learning

https://github.com/cranmer/active_sciencing

AlphaGo

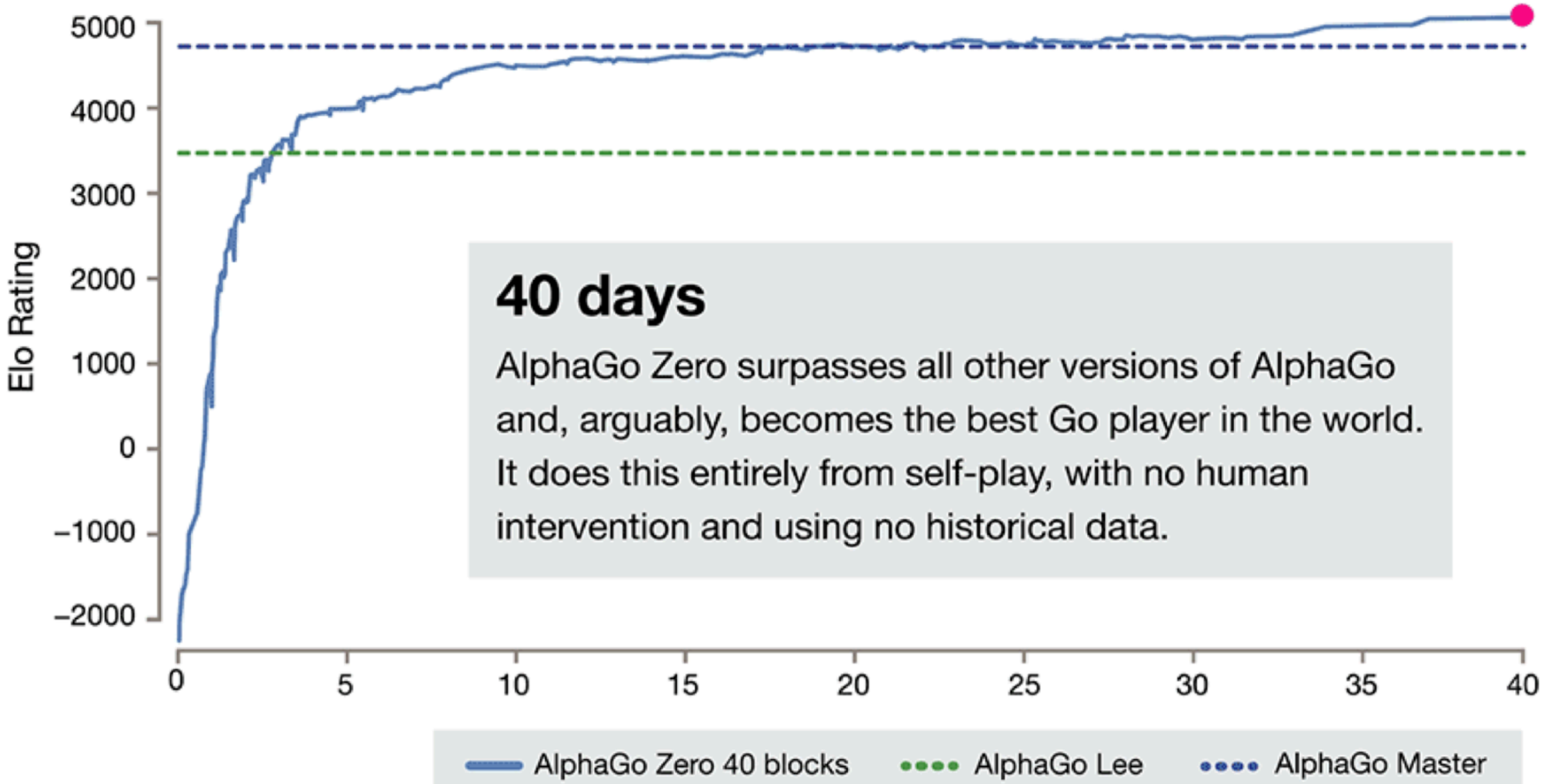


68 at 61

Captured Stones

70 hours

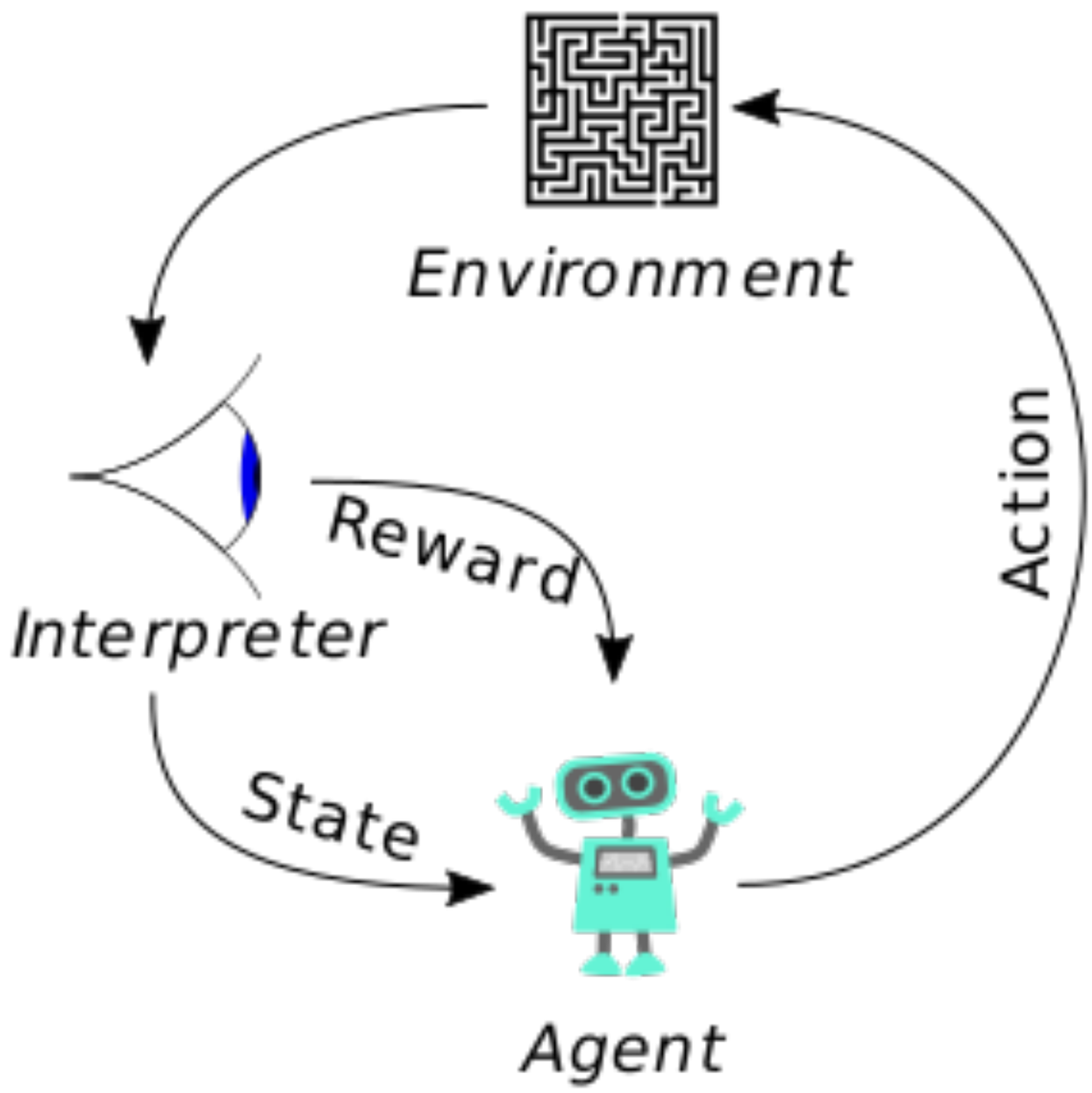
AlphaGo Zero plays at super-human level. The game is disciplined and involves multiple challenges across the board.



40 days

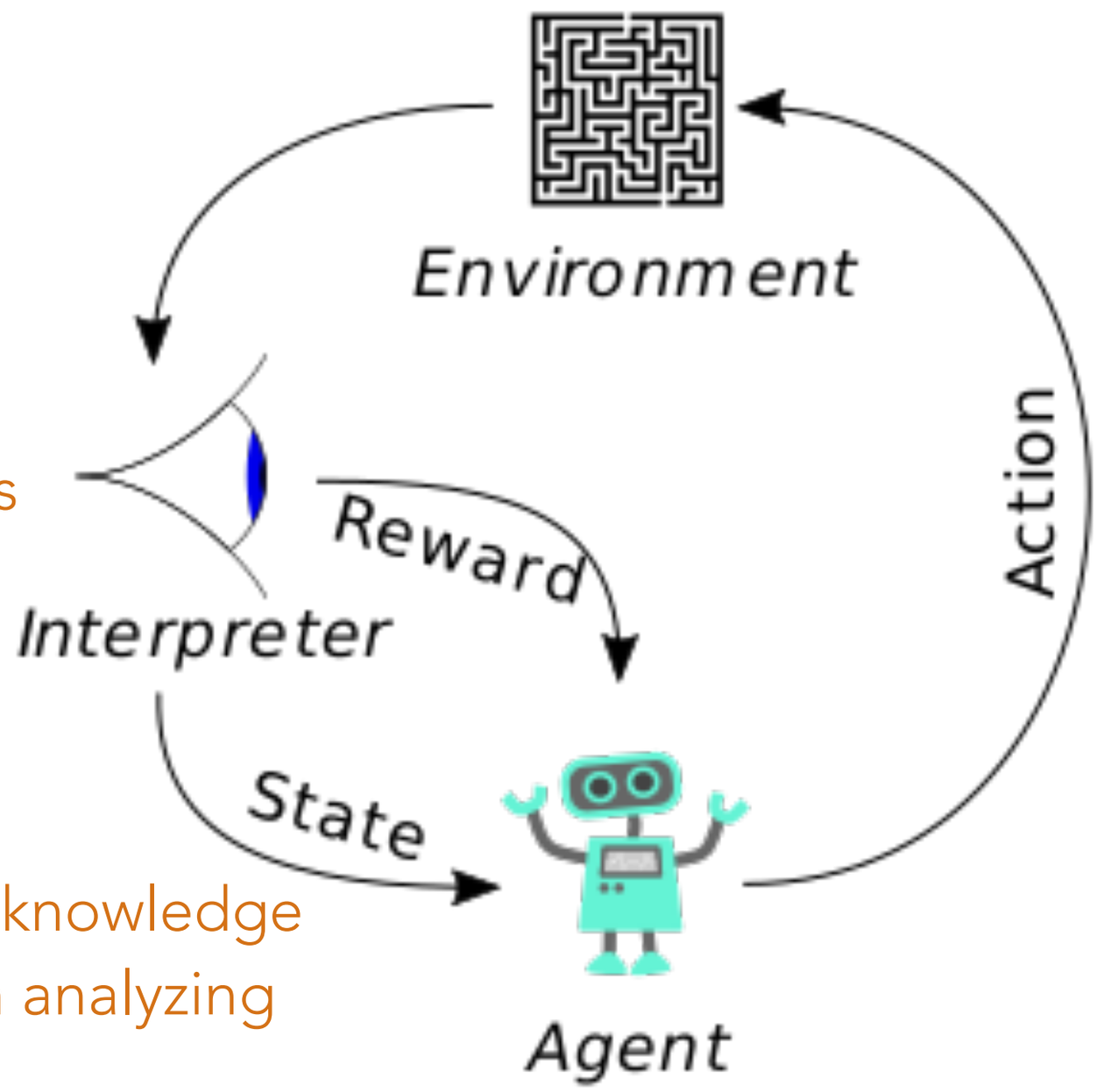
AlphaGo Zero surpasses all other versions of AlphaGo and, arguably, becomes the best Go player in the world. It does this entirely from self-play, with no human intervention and using no historical data.

Scientist trying to decide what experiment to do next



Scientist trying to decide what experiment to do next

perform experiment,
gather data



statistical analysis

decide which
experiment to
perform

updated knowledge
based on analyzing
data

STATISTICAL DECISION THEORY IN 1 SLIDE

Θ - States of nature; X - possible observations; A - action to be taken

$f(x|\theta)$ - statistical model; $\pi(\theta)$ - prior

$\delta: X \rightarrow A$ - **decision rule** (take some action based on observation)

$L: \Theta \times A \rightarrow \mathbb{R}$ - **loss function**, real-valued function true parameter and action

$R(\theta,\delta) = E_{f(x|\theta)}[L(\theta, \delta)]$ - **risk**

- A decision δ^* rule **dominates** a decision rule δ if and only if $R(\theta,\delta^*) \leq R(\theta,\delta)$ for all θ, and the inequality is strict for some θ.

- A decision rule is **admissible** if and only if no other rule dominates it; otherwise it is inadmissible

$r(\pi, \delta) = E_{\pi(\theta)}[R(\theta,\delta)]$ - **Bayes risk** (expectation over θ w.r.t. prior and possible observations)

$\rho(\pi, \delta \mid x) = E_{\pi(\theta|x)}[L(\theta,\delta(x))]$ - **expected loss** (expectation over θ w.r.t. posterior $\pi(\theta|x)$)

- δ' is a (generalized) Bayes rule if it minimizes the expected loss

- under mild conditions every admissible rule is a (generalized) Bayes rule (**with respect to some prior** —possibly an improper one—that favors distributions where that rule achieves low risk). Thus, in frequentist decision theory it is sufficient to consider only (generalized) Bayes rules.

- Conversely, while Bayes rules with respect to proper priors are virtually always admissible, generalized Bayes rules corresponding to improper priors need not yield admissible procedures. Stein's example is one such famous situation.

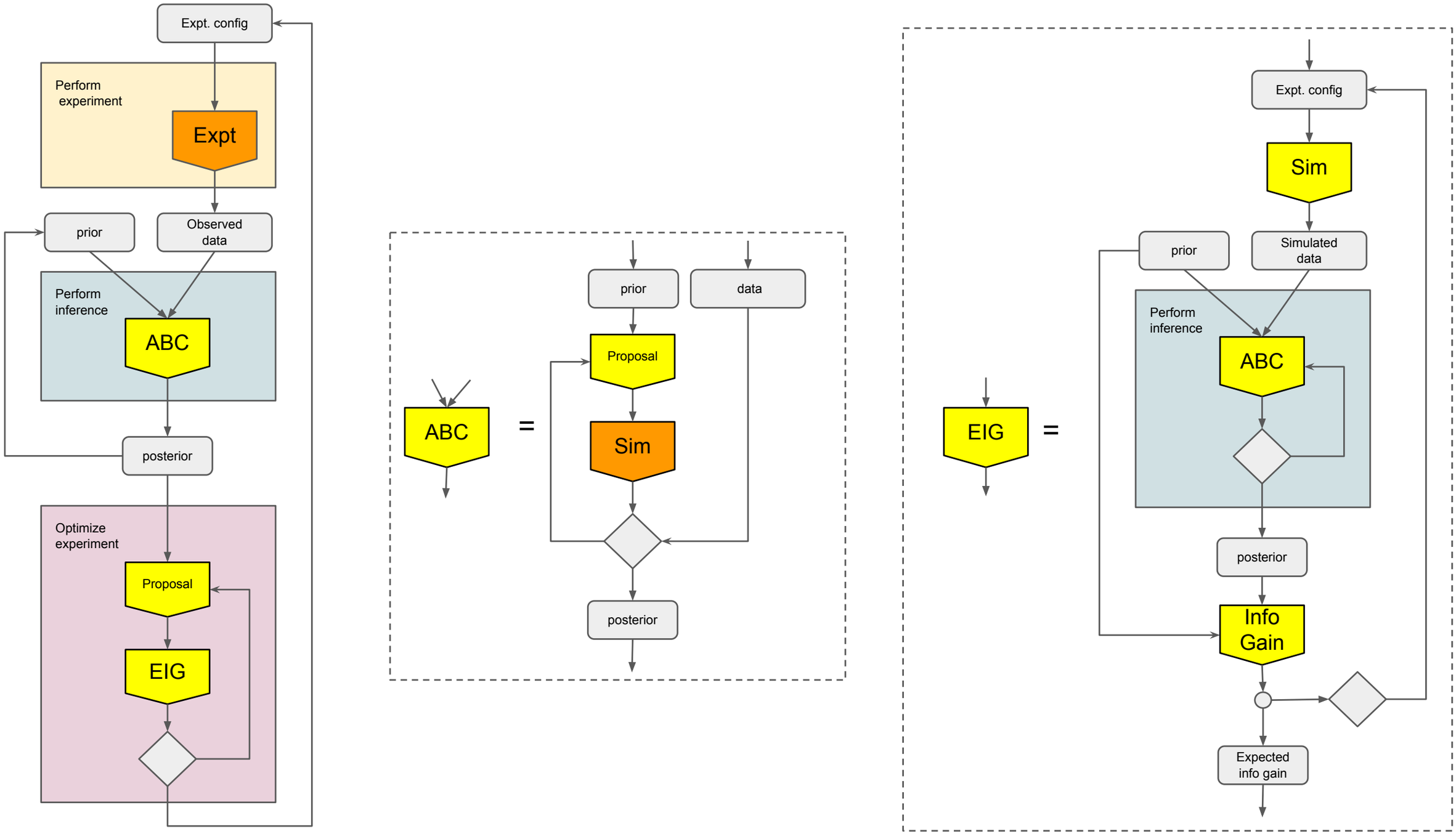
AN EXAMPLE

Say we want to measure the Weinberg angle

- experiments are $e^+e^- \rightarrow \mu^+\mu^-$ at various $\sqrt{s}$ and beam polarization
- data are 4-momenta p_{μ^+} & p_{μ^-} without knowing forward-backward asymmetry is interesting observable

Can we use likelihood-free inference to:

- estimate θ_W from p_{μ^+} & p_{μ^-} generated from simulator?
- **decide** which $\sqrt{s}$ and beam polarization are optimal for this measurement?



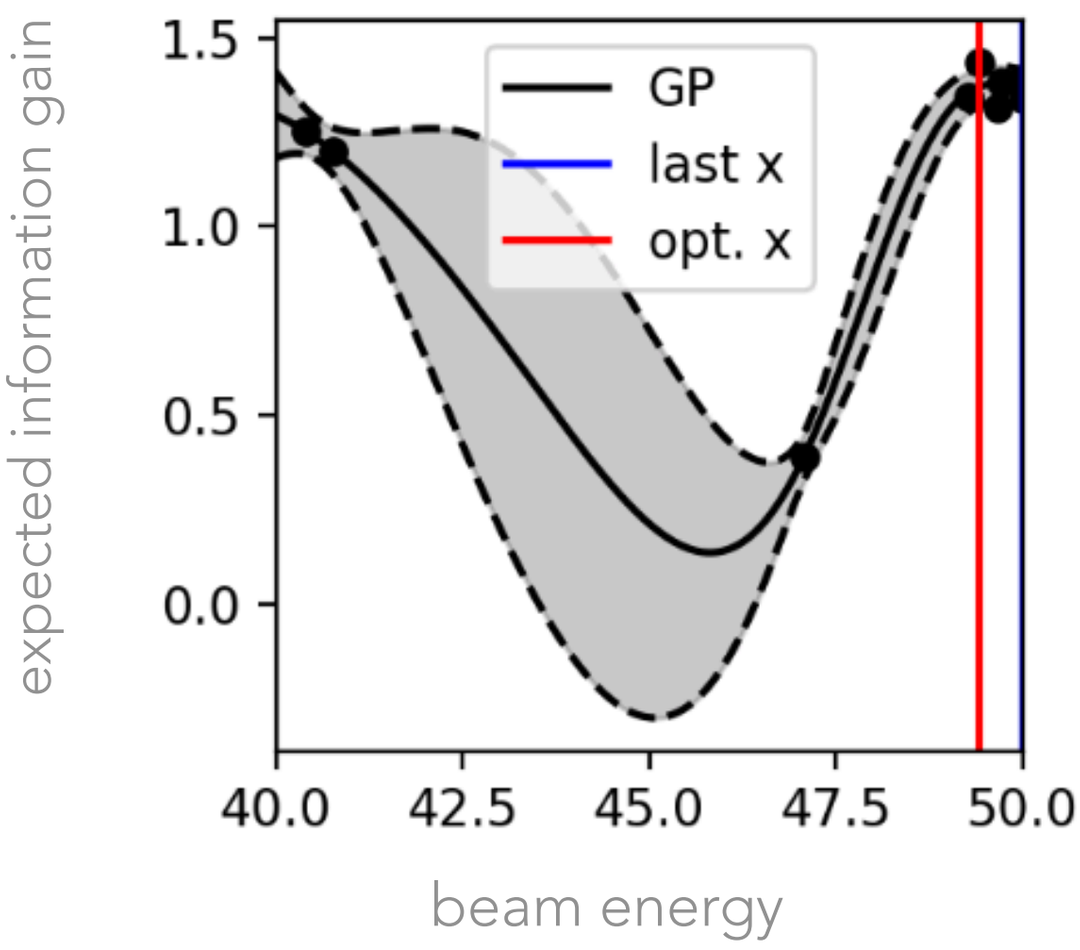
https://github.com/cranmer/active_sciencing

ACTIVE SCIENCING DEMO

Input:

- workflow for performing "real" experiment that returns data
- workflow for running simulator given parameters of theory and experimental configuration

Automated system can measure the Weinberg angle and optimize beam energy (eg. just above or below $M_Z/2$) just from using simulator



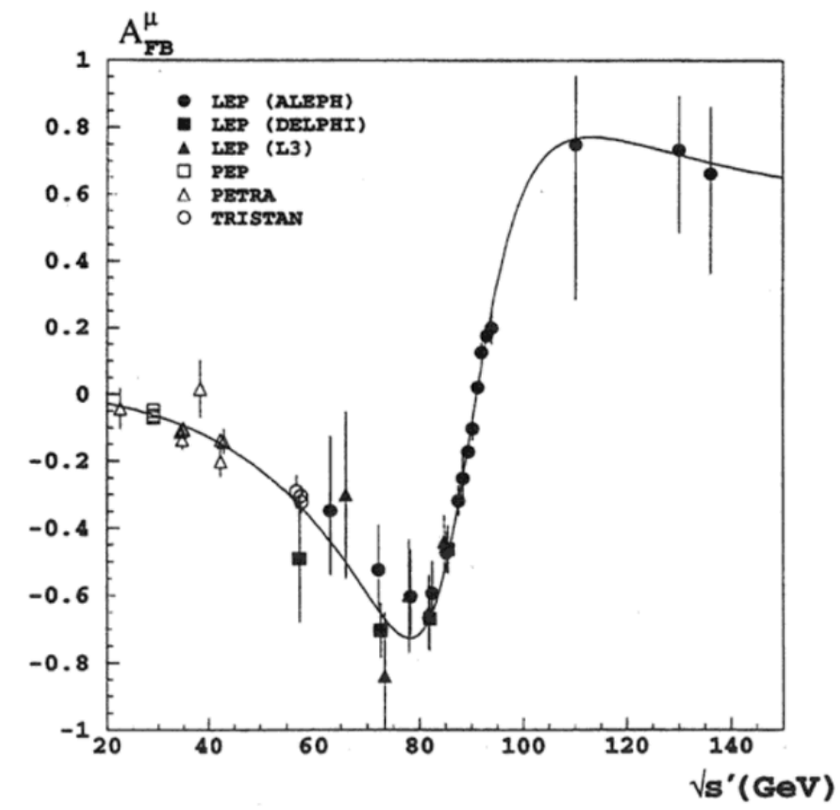


Figure 2: Measured forward-backward asymmetries of muon-pair production compared with the model independent fit results.

CONCLUSIONS

The quest to understand for dark matter will require many different approaches to machine learning

- some cases are plagued with large background uncertainties and have little knowledge of the generative model for the data, we must be more data-driven
- in many cases we want to incorporate relatively vague expert knowledge

Our understanding of how to leverage our prior physics knowledge while letting machine learning do what it's good at is maturing.

- ability to inject and extract physics knowledge from models
- robustness to systematic uncertainty in simulation; training on data

Machine learning also can aid us in exploring the theoretical landscape and in making decisions regarding what data to collect next

MODEL SPECIFICATION

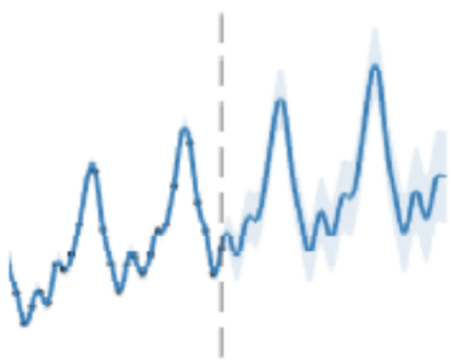
APPROACH	TRACTABLE LIKELIHOOD	SCALABLE TO HIGH DIM. X	COMMENT
SIMULATOR	X	√	MOST DETAILED
ANALYTIC FUNCTION	√	X	AD HOC
HISTOGRAM / TEMPLATE	√	X	TRADITIONAL SURROGATE
NEURAL NETWORK	√	√	PROMISING
GAUSSIAN PROCESS	√	√ (MODERATE)	INCLUDES UNCERTAINTY

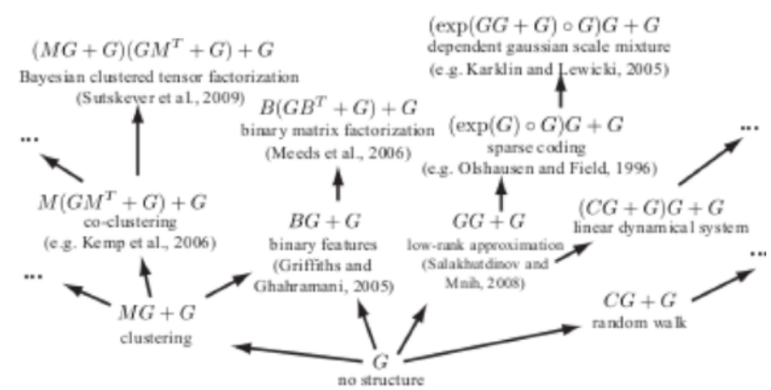
SEARCHING OVER SPACE OF MODELS

Using a class of models known as Gaussian Processes to model data

- physics goes into the construction of a "Kernel" that describes covariance of data

Vocabulary of kernels + grammar for composition





Structure Discovery in Nonparametric Regression through Compositional Kernel Search

David Duvenaud, James Robert Lloyd, Roger Grosse, Joshua B. Tenenbaum, Zoubin Ghahramani

International Conference on Machine Learning, 2013

pdf | code | poster | bibtex

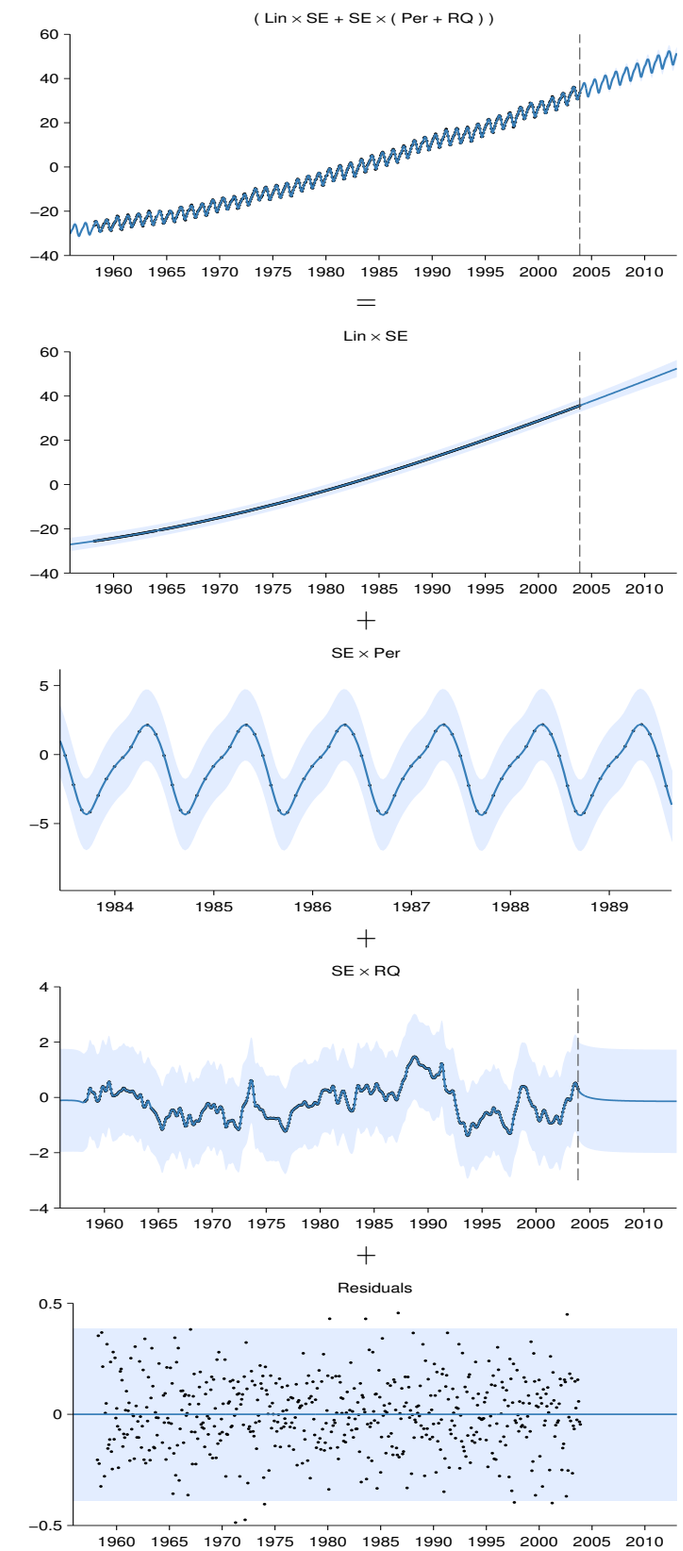
Exploiting compositionality to explore a large space of model structures

Roger Grosse, Ruslan Salakhutdinov, William T. Freeman, Joshua B. Tenenbaum

Conference on Uncertainty in Artificial Intelligence, 2012

pdf | code | bibtex

Mauna Loa atmospheric CO_2



Better Simplified Likelihoods

Cranmer, Kreiss, Lopez-Val, Plehn
https://arxiv.org/abs/1401.0080

SIMPLIFIED LIKELIHOODS

CMS NOTE -2017/001

elled by modifying the background contributions as $b_i \to b_i + \theta_i$. The probability to simultaneously observe each of the n_i events in N search regions is the product of probabilities across the search regions such that

$$\mathcal{P}(\text{data}|\mu \cdot s(\boldsymbol{\theta}) + b(\boldsymbol{\theta})) = \prod_{i=1}^{N} P(n_i|\mu \cdot s_i + b_i + \theta_i). \tag{3}$$

Some simplifying assumptions must be made in order to reduce the complexity of the full probability density function $p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})$.

- The constraints on the background contributions are Gaussian such that the distribution of the number of background events is symmetric about the expectation, b_i, and its variance is independent of $\boldsymbol{\theta}$. Often, the background contributions are estimated from control regions in data with large sample sizes, which makes this assumption valid.
- The covariance, and therefore only the linear correlation, between the background contribution in each region is sufficient to approximate $p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})$ at least for values of $\boldsymbol{\theta}$ which are close to $\tilde{\boldsymbol{\theta}}$.
- The numbers of events, n_i, are statistically independent from one another. This is true when there are no events which are included in more than one search region and the estimates of the background contributions, b_i, and covariance matrix $\mathbf{V}$ have not been obtained from data which are statistically dependent on the data from any search region.
- The systematic uncertainties in the signal model can be neglected. The validity of this assumption will strongly depend on the specific BSM physics model being considered. Systematic uncertainties on the signal can be accounted for by adding appropriate nuisance parameters with Gaussian constraints as for the background contributions.

Under these assumptions, $p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})$ can be modelled as a multivariate Gaussian distribution with the mean vector identified with external measurements of $\tilde{\boldsymbol{\theta}} = 0$. The simplified likelihood can now be expressed as

$$\mathcal{L}_S(\mu, \boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{(\mu \cdot s_i + b_i + \theta_i)^{n_i} e^{-(\mu \cdot s_i + b_i + \theta_i)}}{n_i!} \cdot \exp\left(-\frac{1}{2}\boldsymbol{\theta}^T \mathbf{V}^{-1} \boldsymbol{\theta}\right), \tag{4}$$

where $\mathbf{V}$ represents the covariance matrix for the expected background contributions across the search regions and is defined as

$$V_{ij} = E[\theta_i \times \theta_j], \tag{5}$$

where $E[x]$ is the expectation value of x.

For the results shown for the following example, the simplified likelihood is constructed using the statistics package ROOFIT [16] but it should be noted that the procedure does not prohibit the use of any other tool for its construction.

Looks familiar:

Phys.Rev. D91 (2015) no.5, 054032 arXiv:1401.0080

Decoupling Theoretical Uncertainties from Measurements of the Higgs Boson

Kyle Cranmer[1], Sven Kreiss[1], David López-Val[2], and Tilman Plehn[3]
[1] *Center for Cosmology & Particle Physics, New York University, USA*
[2] *Centre for Cosmology, Particle Physics & Phenomenology, Université Catholique de Louvain, Belgium and*
[3] *Institut für Theoretische Physik, Universität Heidelberg, Germany*

$$L_{\text{full}}(\boldsymbol{\mu}, \boldsymbol{\alpha}) = \underbrace{\prod_{c \in \text{category}} \left[\text{Pois}(n_c|\nu_c(\boldsymbol{\mu}, \boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_e|\boldsymbol{\mu}, \boldsymbol{\alpha}) \right]}_{\equiv L_{\text{main}}(\boldsymbol{\mu}, \boldsymbol{\alpha})} \underbrace{\prod_{i \in \text{syst}} f_i(a_i|\alpha_i)}_{\equiv L_{\text{constr}}(\boldsymbol{\alpha})} . \tag{4}$$

Typically, confidence intervals are then defined by contours of the profile likelihood ratio

$$\lambda(\boldsymbol{\mu}) = \frac{L(\boldsymbol{\mu}, \hat{\hat{\alpha}}(\boldsymbol{\mu}))}{L(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\alpha}})} \tag{5}$$

where $\hat{\hat{\boldsymbol{\alpha}}}(\boldsymbol{\mu})$ is the conditional maximum likelihood estimate and $\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\alpha}}$ are the unconditional maximum likelihood estimates [19].

B. The Effective Signal Strength

We are interested in inferring the values of the signal strength parameters $\boldsymbol{\mu}$, which scale the signal expectation s_{cpd}; however, the presence of experimental and theoretical uncertainties mean that the signal and background expectations are functions of the nuisance parameters as in Eq.(2). Alternatively, we can introduce effective scale factor with respect to some fixed reference scenario $\boldsymbol{\alpha}_0$, so the expected number of events can be re-written

$$\begin{aligned} \nu_c(\boldsymbol{\mu}, \boldsymbol{\alpha}) &= \sum_{p,d} \mu_{pd}\, s_{cpd}(\boldsymbol{\alpha}) + b_c(\boldsymbol{\alpha}) \\ &\to \sum_{p,d} \mu^{\text{eff}}_{cpd}(\boldsymbol{\mu}, \boldsymbol{\alpha})\, s_{cpd}(\boldsymbol{\alpha}_0) + b_c(\boldsymbol{\alpha}_0) . \end{aligned} \tag{6}$$

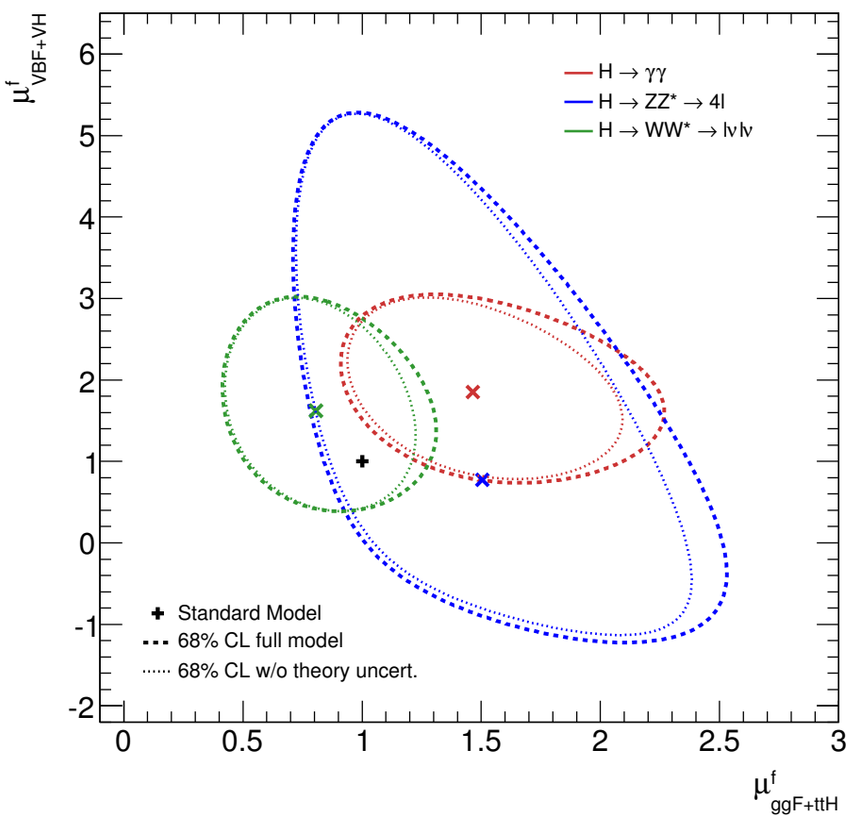
- equivalent if you make simplifying assumptions
- but this approach doesn't need assumptions 1,2, or 4

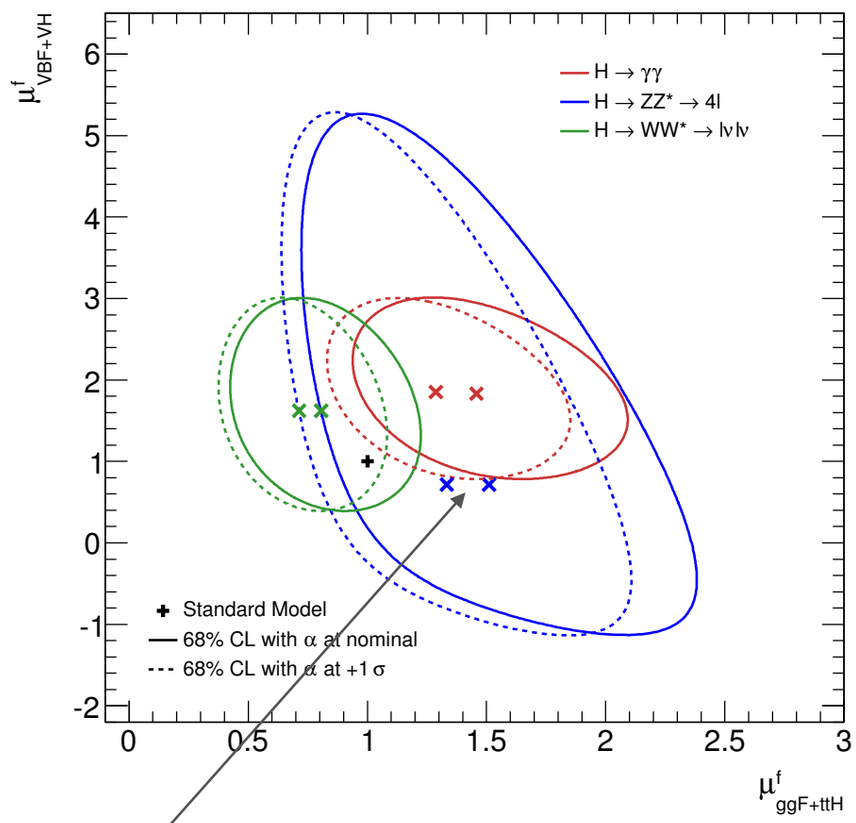
Basic idea (1/2)

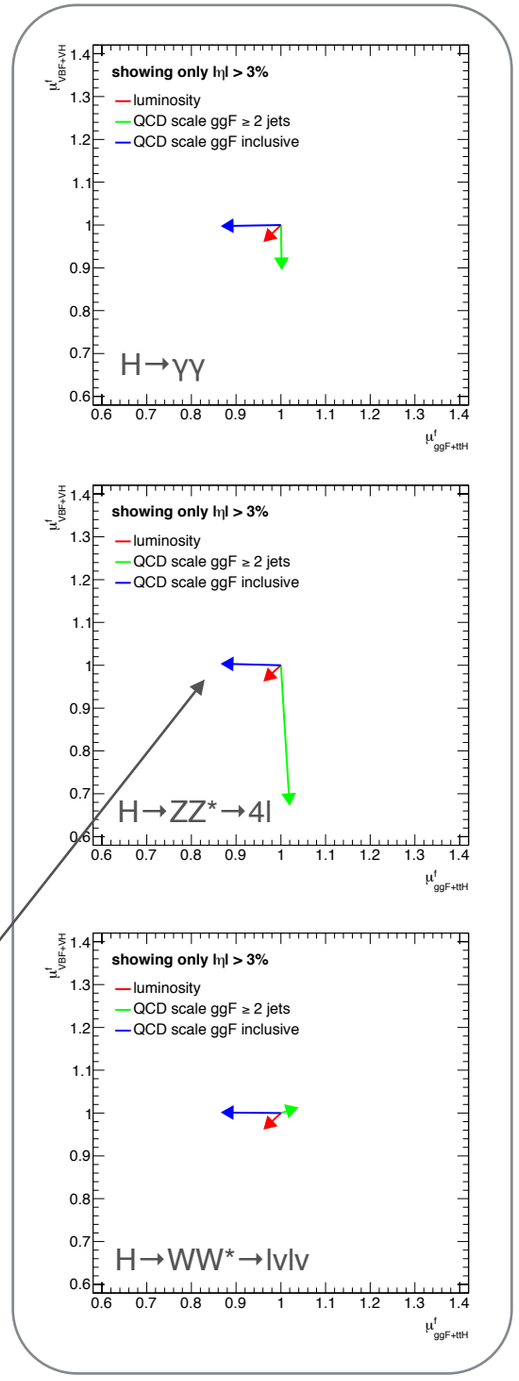
Left: contours with / without theory uncertainties

Center: contours w/o theory uncertainty shifted by changing ggF inclusive x-sec up by 1σ

Right: collection of vectors indicating how best fit point moves due to each source of uncertainty







All plots are based on counting models that mimic ATLAS results.

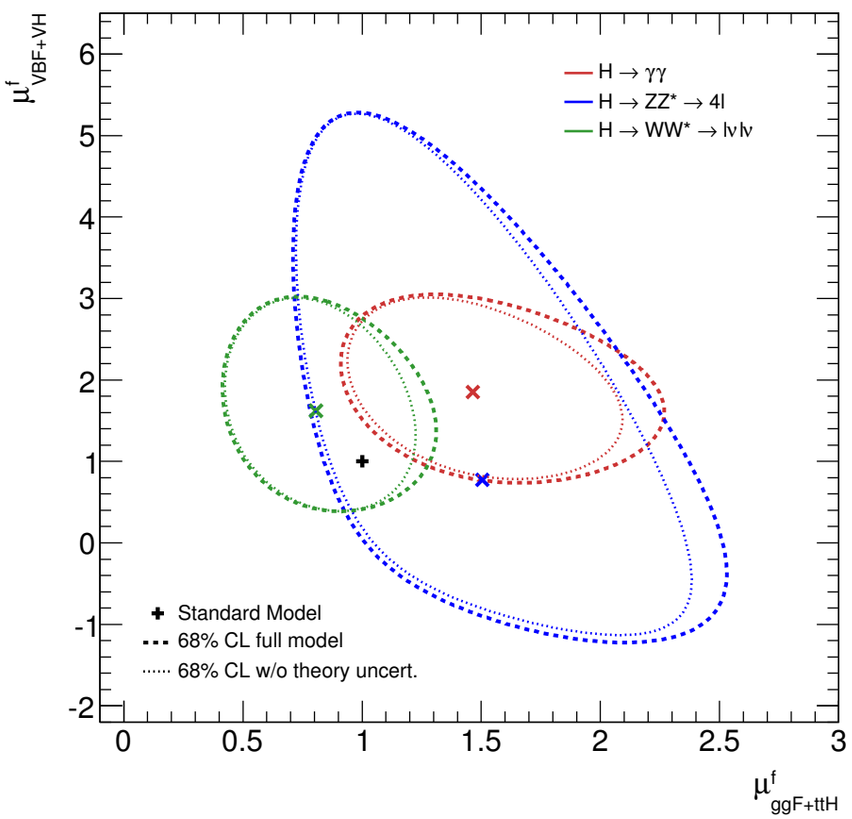
Points move in this plane when varying **common nuisance parameters.**

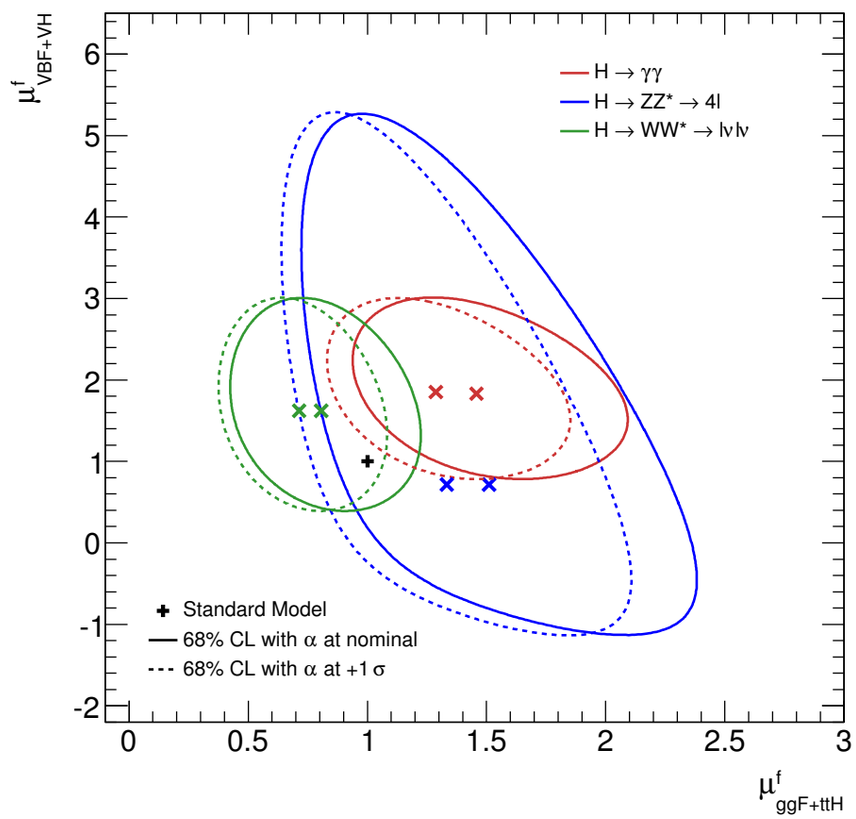
$$\left.\frac{\partial \hat{\mu}_p^{\text{fix}}}{\partial \alpha_i}\right|_{\hat{\boldsymbol{\mu}},\hat{\boldsymbol{\alpha}}} = -\hat{\mu}_p \eta_{ip}$$

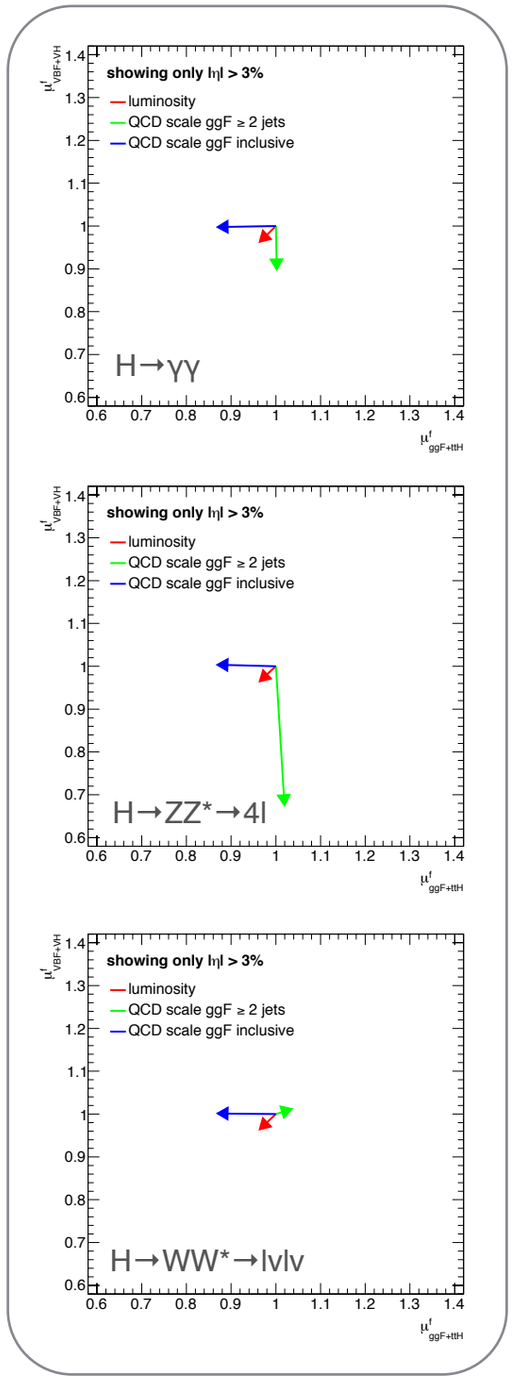
Basic idea (2/2)

Basic idea: Instead of folding the theoretical uncertainties into the experimental result, experiments would publish an **effective likelihood** $L_{\mathrm{eff}}(\mu^{\mathrm{eff}})$ with respect to some fixed theoretical reference and a **reparametrization template** $\mu^{\mathrm{eff}}(\mu,\alpha)$ that documents the affect of individual sources of uncertainty.

theoretical uncertainties are **decoupled** from experimental result!





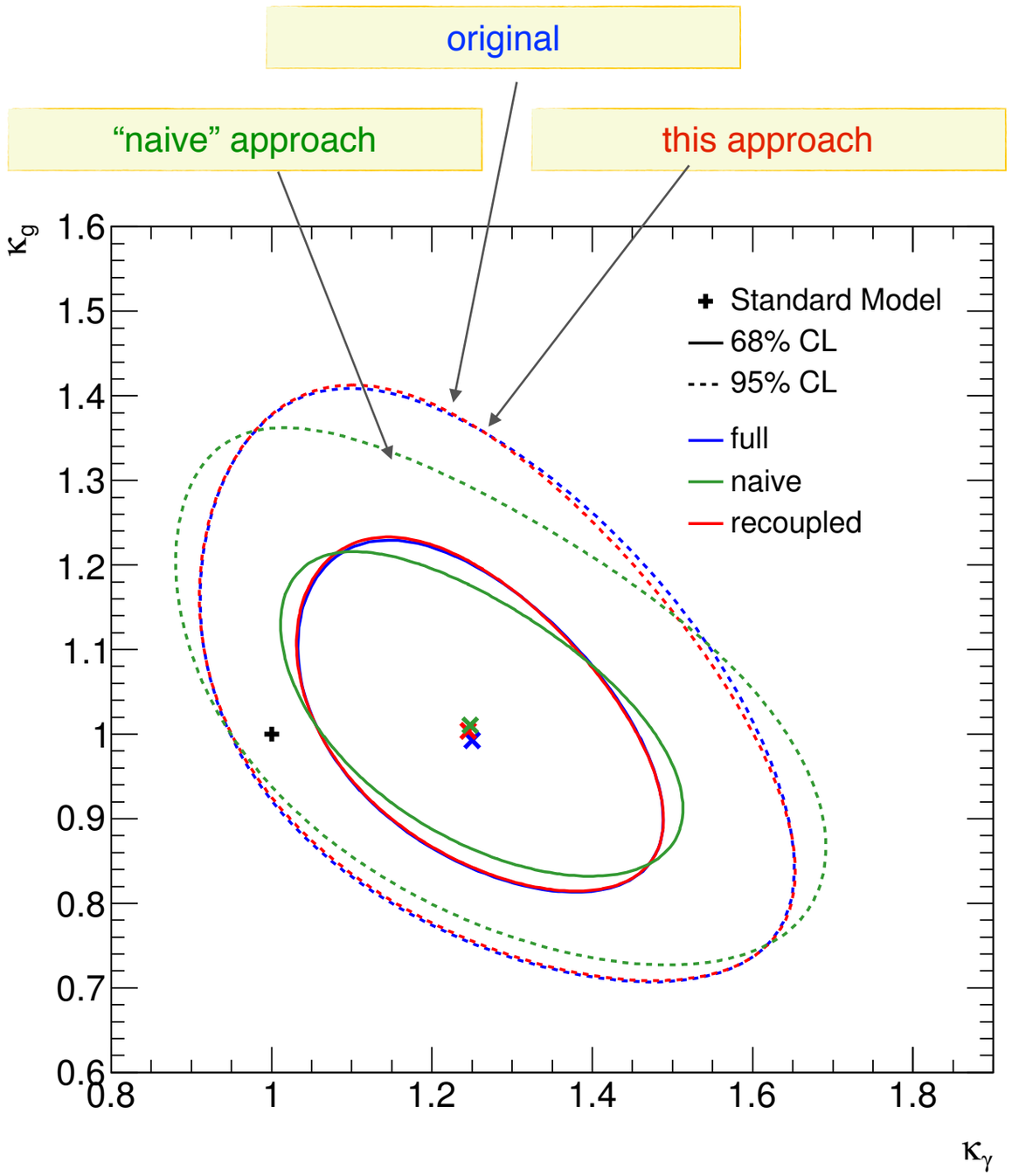


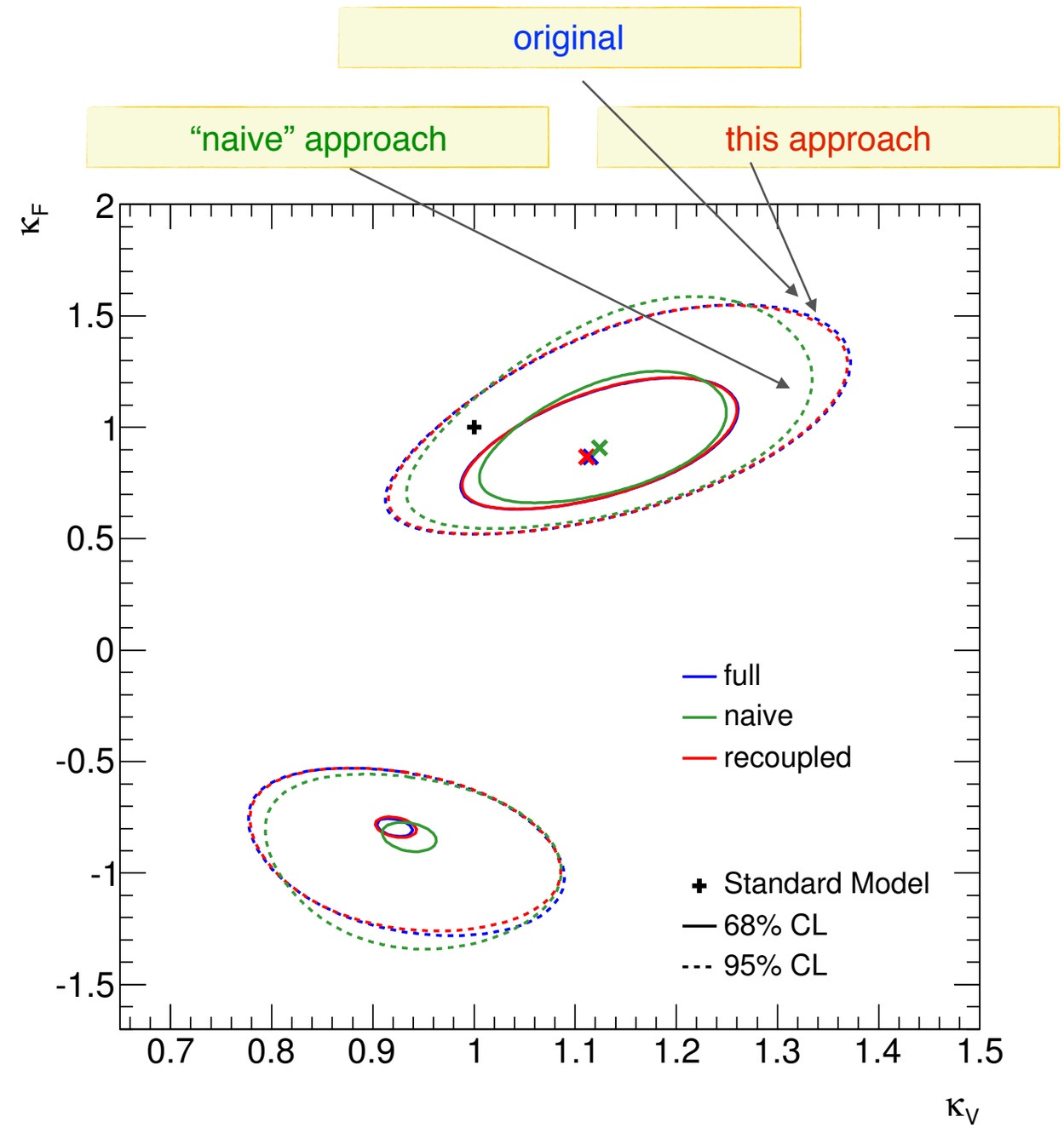
Then the full likelihood (left) can be **recoupled** by composition and one is free to modify the constraint term (prior)

$$L_{\mathrm{full}}(\boldsymbol{\mu},\boldsymbol{\alpha}) \approx L_{\mathrm{recouple}}(\boldsymbol{\mu},\boldsymbol{\alpha}) \equiv L_{\mathrm{eff}}(\boldsymbol{\mu}^{\mathrm{eff}}(\boldsymbol{\mu},\boldsymbol{\alpha})) \cdot L_{\mathrm{constr}}(\boldsymbol{\alpha})$$

Results with combined Higgs benchmark

Here are results for two Higgs coupling benchmark models





All plots are based on counting models that mimic ATLAS results.

A toy example with large uncertainties

Three examples for a simple 2 channel case with large uncertainties.

The recoupled likelihood excellent approximation to full likelihood

Contour with no theory uncertainty much smaller

Contour with theory uncertainty much larger. Here treated using Gaussian constraint term (prior)

Modified contour switching from Gaussian to RFIT / box constraint.

Anyone can do in recoupled approach, but would require a experiments to re-run in current approach.

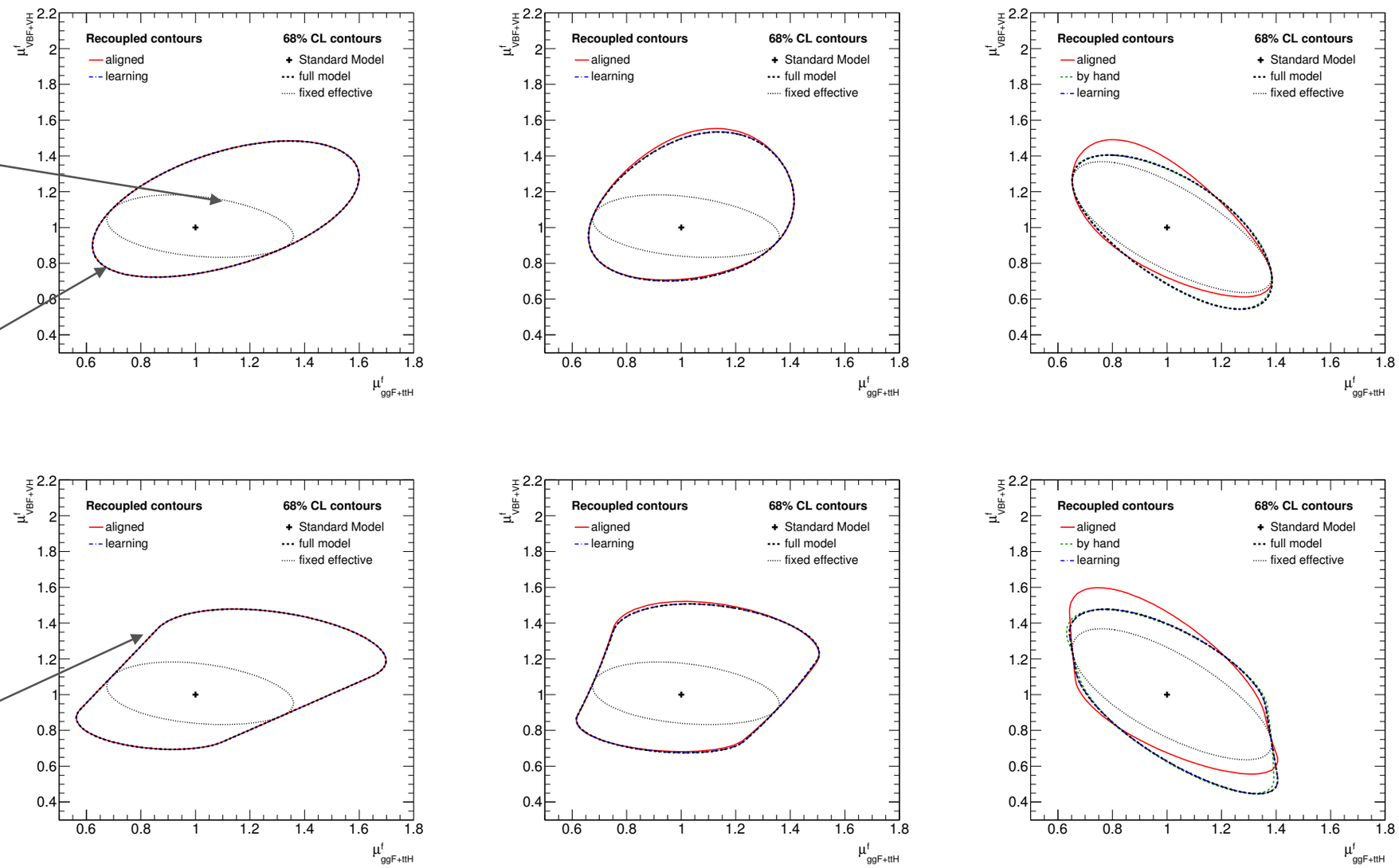


Figure 7. Comparison of full likelihood (solid) and recouped (dashed) likelihood for Scenarios A, B, and C. Scenario C illustrates the impact of using three templates 'aligned' (red), 'by hand' (green), and 'learning' (blue) as described in the text. The top row is based on the nominal Gaussian constraint and the bottom row shows the result of replacing it with an alternative RFIT constraint term. The effective likelihood with $\alpha = 0$ is shown as a dotted line.

CONNECTION TO MACHINE LEARNING

The heart of the method is to learn a "reparametrization template" $\mu_{\text{eff}}(\mu,\boldsymbol{\alpha})$ that says how likelihood on parameters of interest is deformed by changes to other parameters

$$L_{\text{full}}(\boldsymbol{\mu},\boldsymbol{\alpha}) \approx L_{\text{recouple}}(\boldsymbol{\mu},\boldsymbol{\alpha}) \equiv L_{\text{eff}}(\boldsymbol{\mu}^{\text{eff}}(\boldsymbol{\mu},\boldsymbol{\alpha})) \cdot L_{\text{constr}}(\boldsymbol{\alpha})$$

- We can use use machine learning techniques to learn this reparametrization template

c. Via a global learning approach Ideally we would have a formalism that would work with the black box likelihood $L_{\text{full}}(\boldsymbol{\mu},\boldsymbol{\alpha})$ and a general template like Eq.(13) without having to introduce by hand restrictions on that template as described above. In order to do that we must introduce information about the likelihood away from $(\hat{\boldsymbol{\mu}},\hat{\boldsymbol{\alpha}})$. A flexible approach to that problem is based on the ideas of machine learning and function approximation in which one aims to minimize a loss function with respect to some model parameters (in this case the template coefficients). The loss function needs to be a scalar evaluated over the $(\boldsymbol{\mu},\boldsymbol{\alpha})$ space, which in frequentist terms has no measure. However, from the point of view of decision theory, one can introduce some weighting over the parameter space (without regarding it as a Bayesian prior) and evaluate

$$\text{Loss}(\boldsymbol{\eta}) = \int d\boldsymbol{\mu} d\boldsymbol{\alpha}\, \pi(\boldsymbol{\mu},\boldsymbol{\alpha})\, \left|L_{\text{full}}(\boldsymbol{\mu},\boldsymbol{\alpha}) - L_{\text{recouple}}(\boldsymbol{\mu},\boldsymbol{\alpha};\boldsymbol{\eta})\right|^2 \tag{27}$$

Why should physicists care?

THE PLAYERS

forward modeling
generation
simulation

PREDICTION

θ
parameters of interest

$p(x, z \mid \theta, \nu)$

x
observed data
simulated data

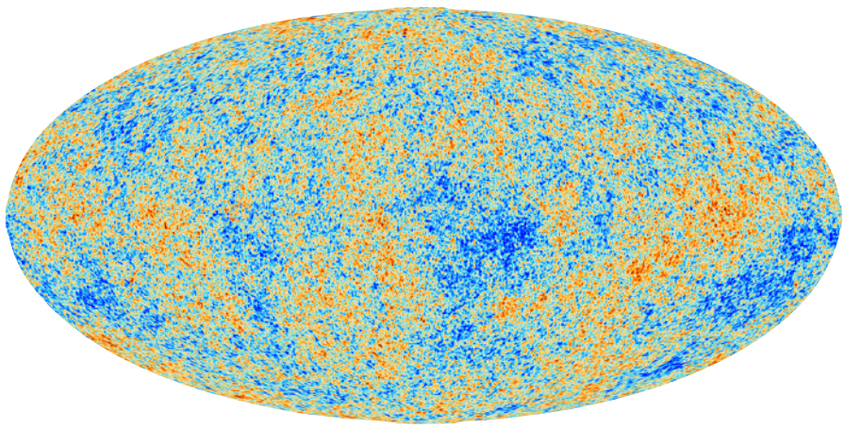
z
latent variables
Monte Carlo truth

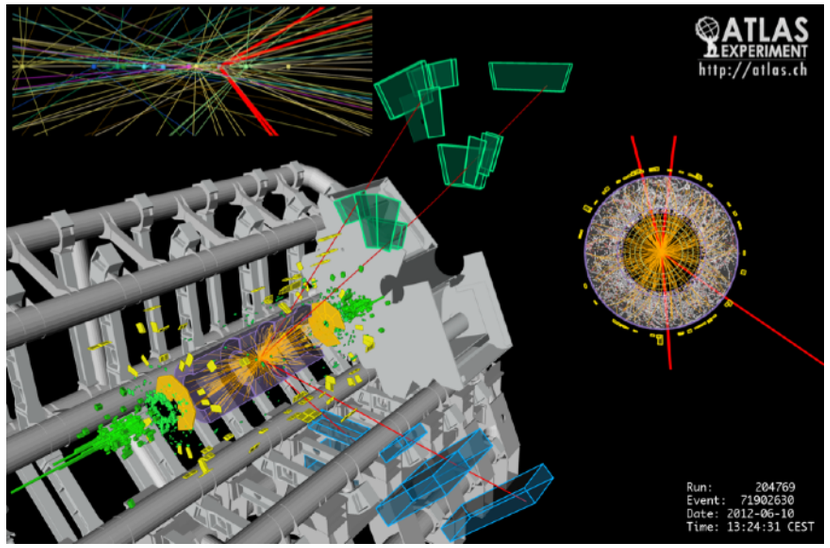
ν
nuisance parameters

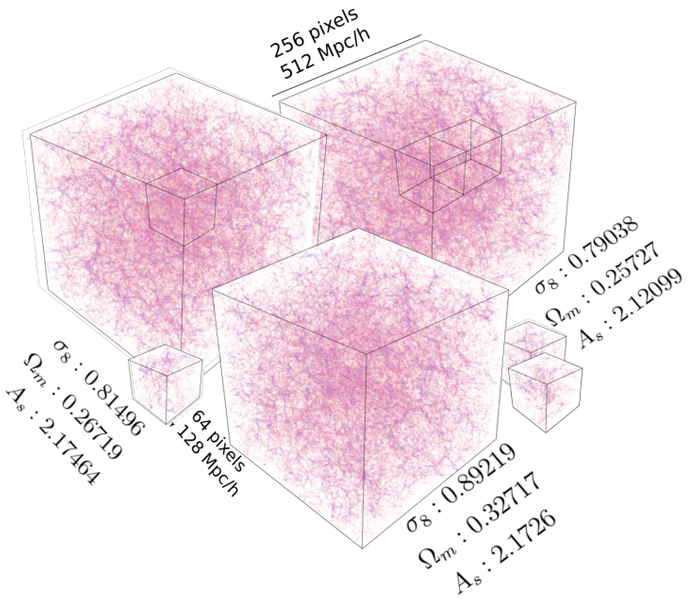
INFERENCE

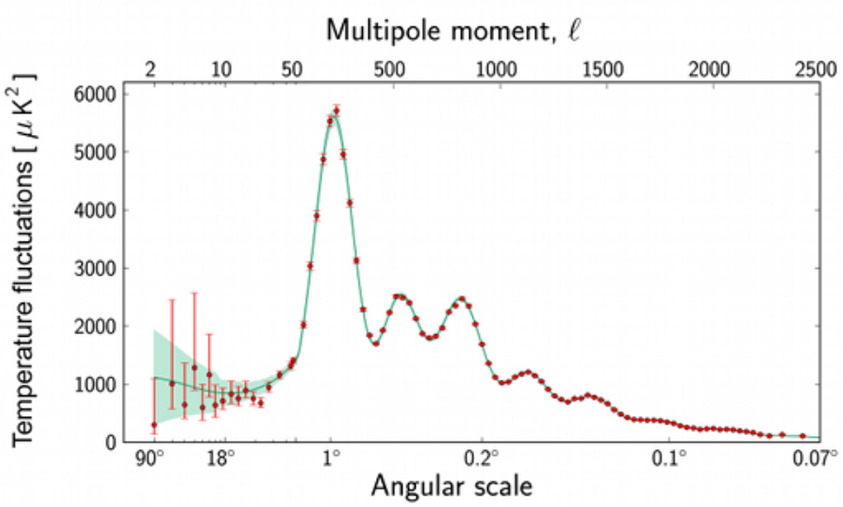
inverse problem
measurement
parameter estimation

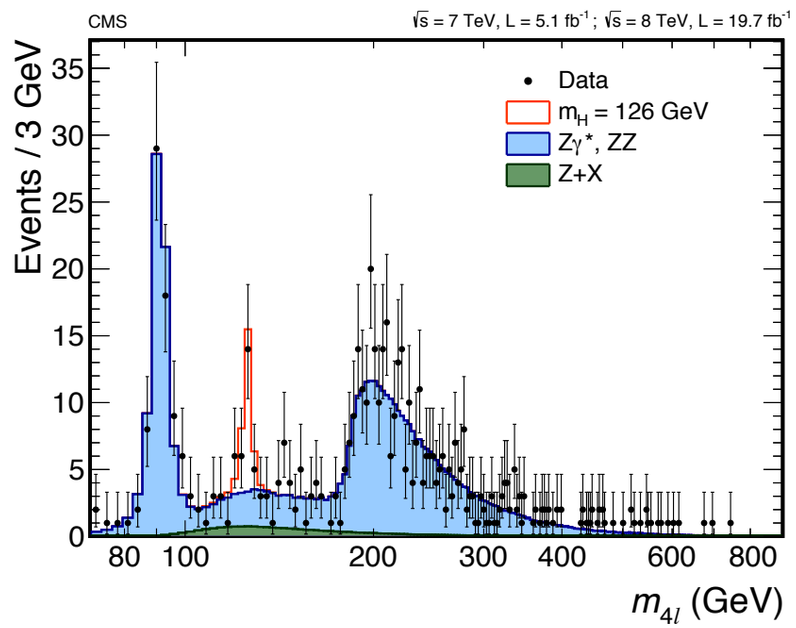
PREDICTION: THE FORWARD MODEL

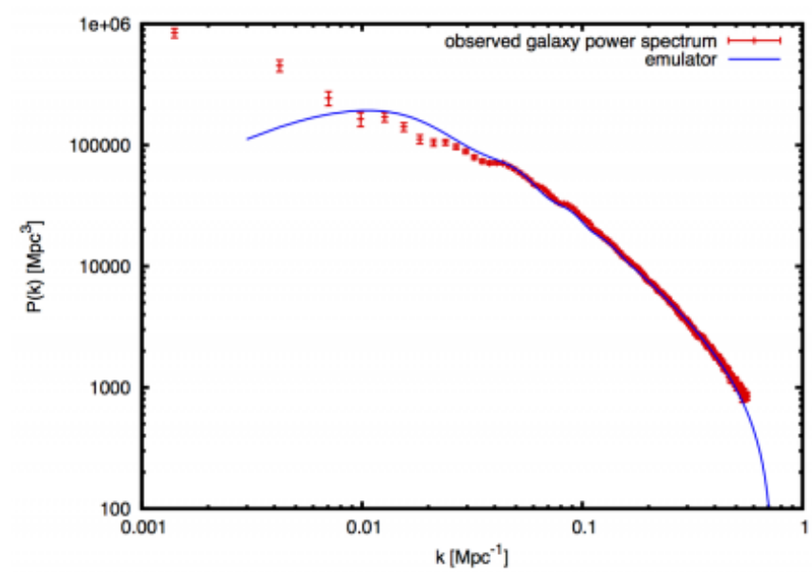












WHY WE SHOULD CARE

Many areas of science have simulations based on some well-motivated mechanistic model.

However, the aggregate effect of many interactions between these low-level components leads to an intractable inverse problem.

The developments in machine learning and AI go way beyond improved classifiers and have the potential to effectively bridge the microscopic - macroscopic divide & aid in the inverse problem.

- they can provide effective statistical models that describe macroscopic phenomena that are tied back to the low-level microscopic (reductionist) model
- generative models and likelihood-free inference are two particularly exciting areas

Physics-Aware Machine Learning:

"There is great promise at the interface of physical models and data driven models."

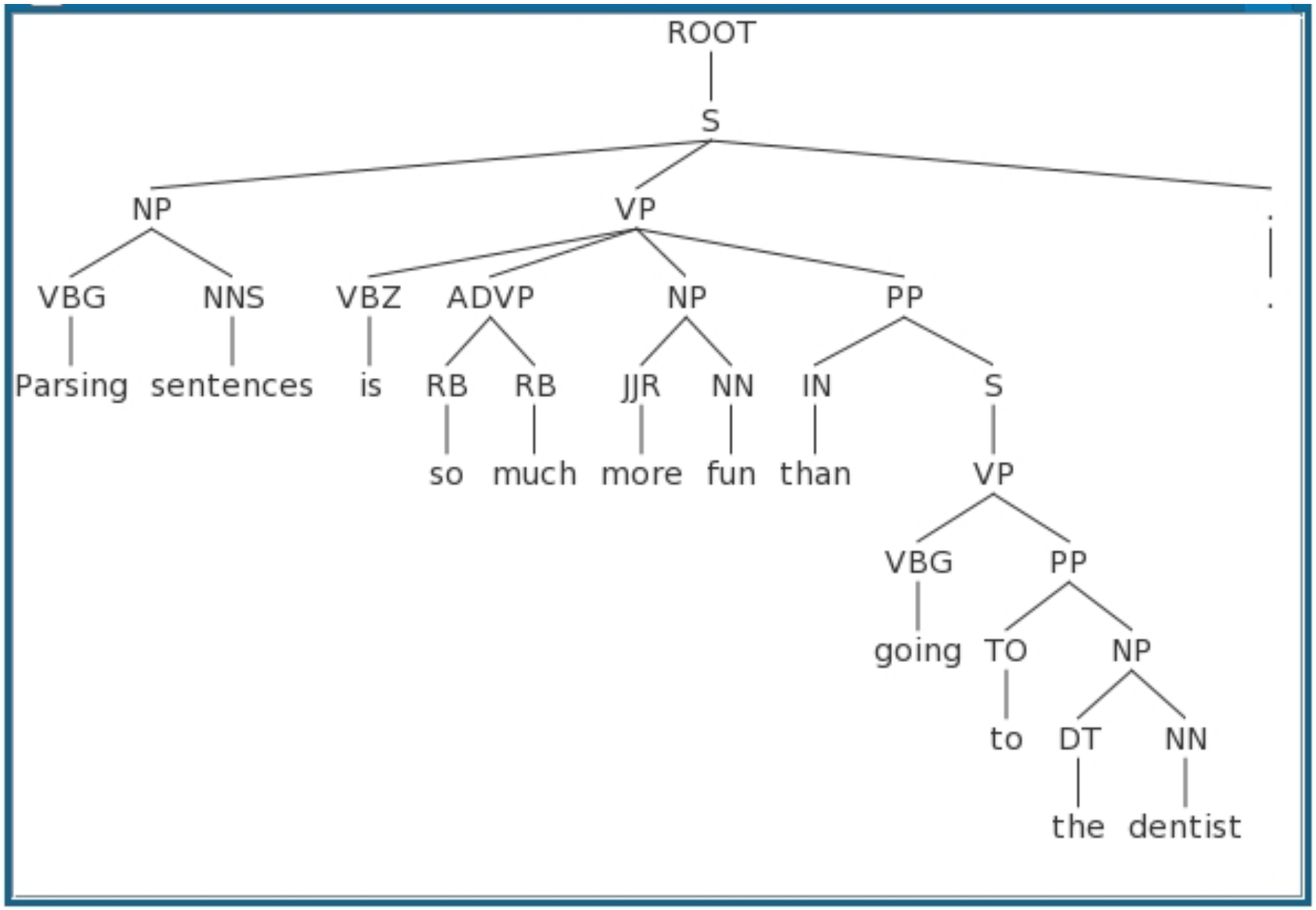
–NEIL LAWRENCE

http://inverseprobability.com/2016/11/29/new-directions-in-kernels-and-gaussian-processes.html

FROM IMAGES TO SENTENCES

Recursive Neural Networks showing great performance for Natural Language Processing tasks

- neural network's topology given by parsing of sentence!



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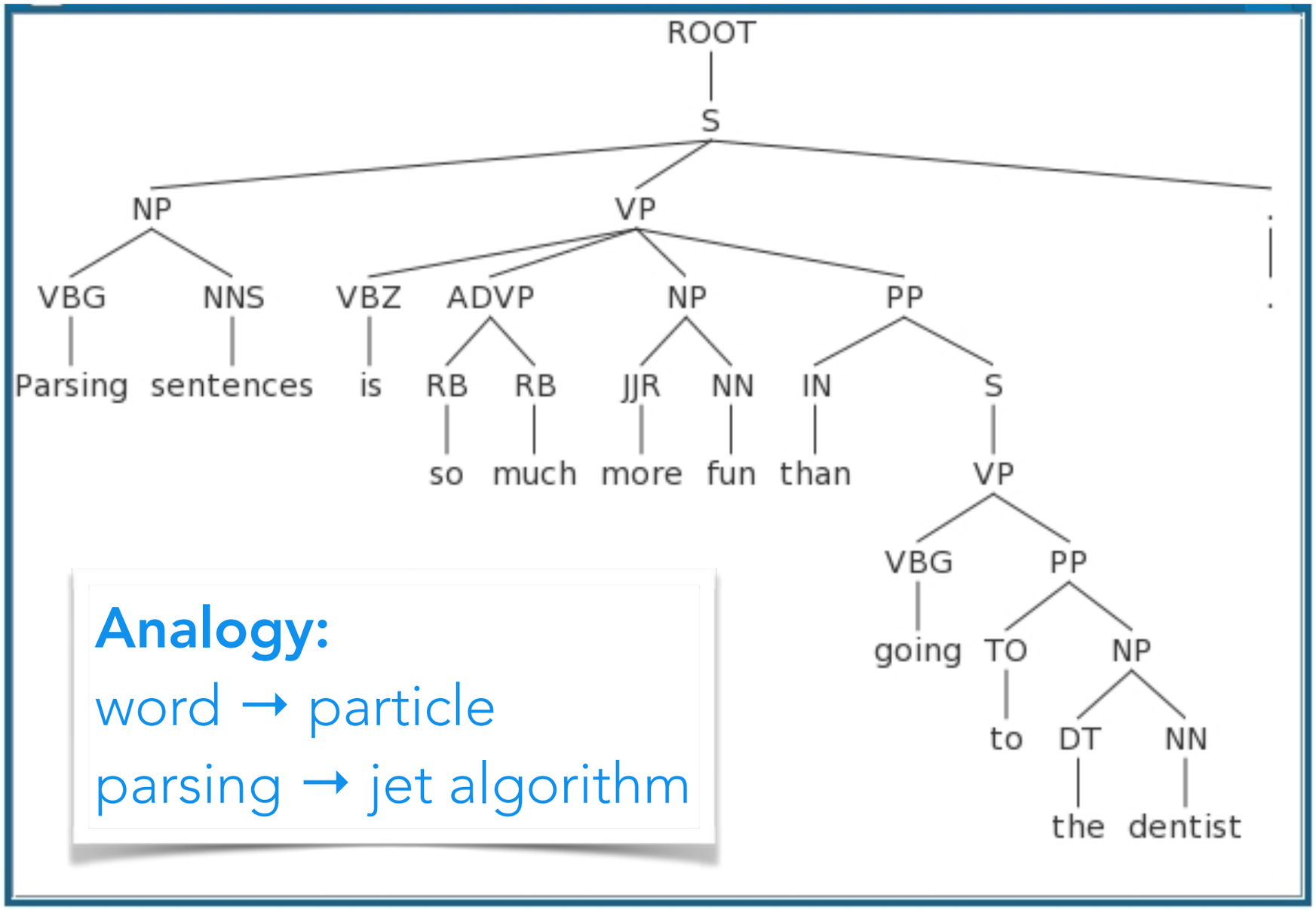
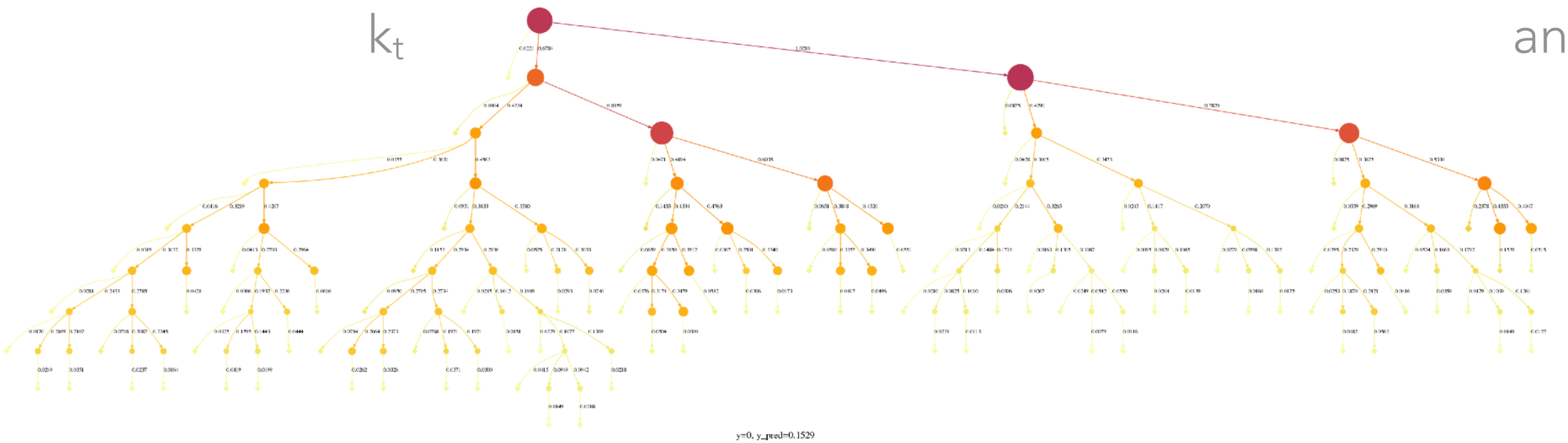


Analogy:
word → particle
parsing → jet algorithm

QCD-INSPIRED RECURSIVE NEURAL NETWORKS



Work with Gilles Louppe, Kyunghyun Cho, Cyril Becot

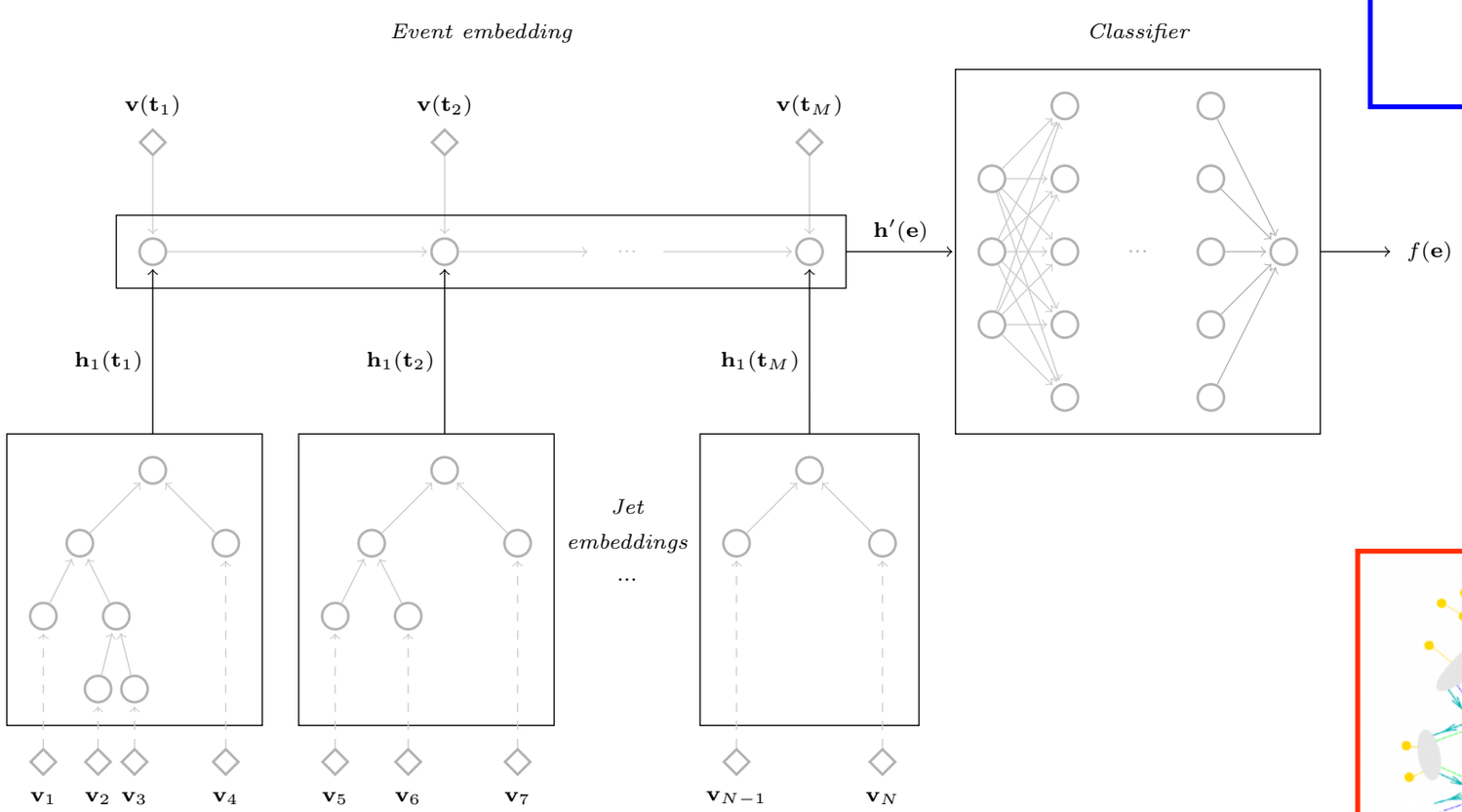
- Use sequential recombination jet algorithms to provide network topology (on a per-jet basis)
- path towards ML models with good physics properties
- Top node of recursive network provides a fixed-length **embedding** of a jet that can be fed to a classifier

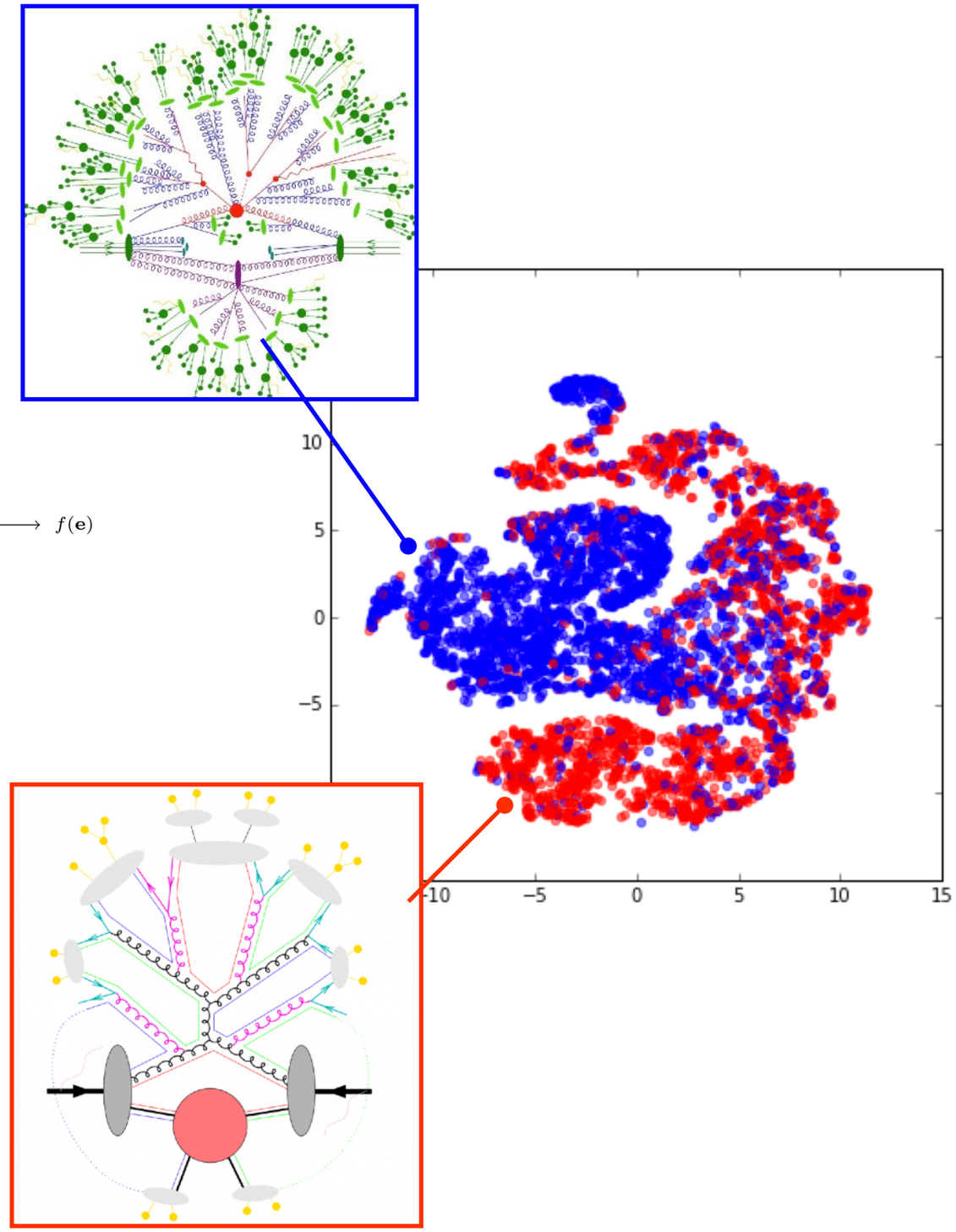
arXiv:1702.00748 & follow up work with Joan Bruna using graph conv nets

JOINTLY OPTIMIZE HIERARCHICAL MODEL

particle embedding → jet embedding → event embedding → classifier

It scales!





arXiv:1702.00748

Reconstruction as a Structured Inverse Problem

(Monte Carlo Truth = Latent Variables)

"LA MIA PARABOLA"

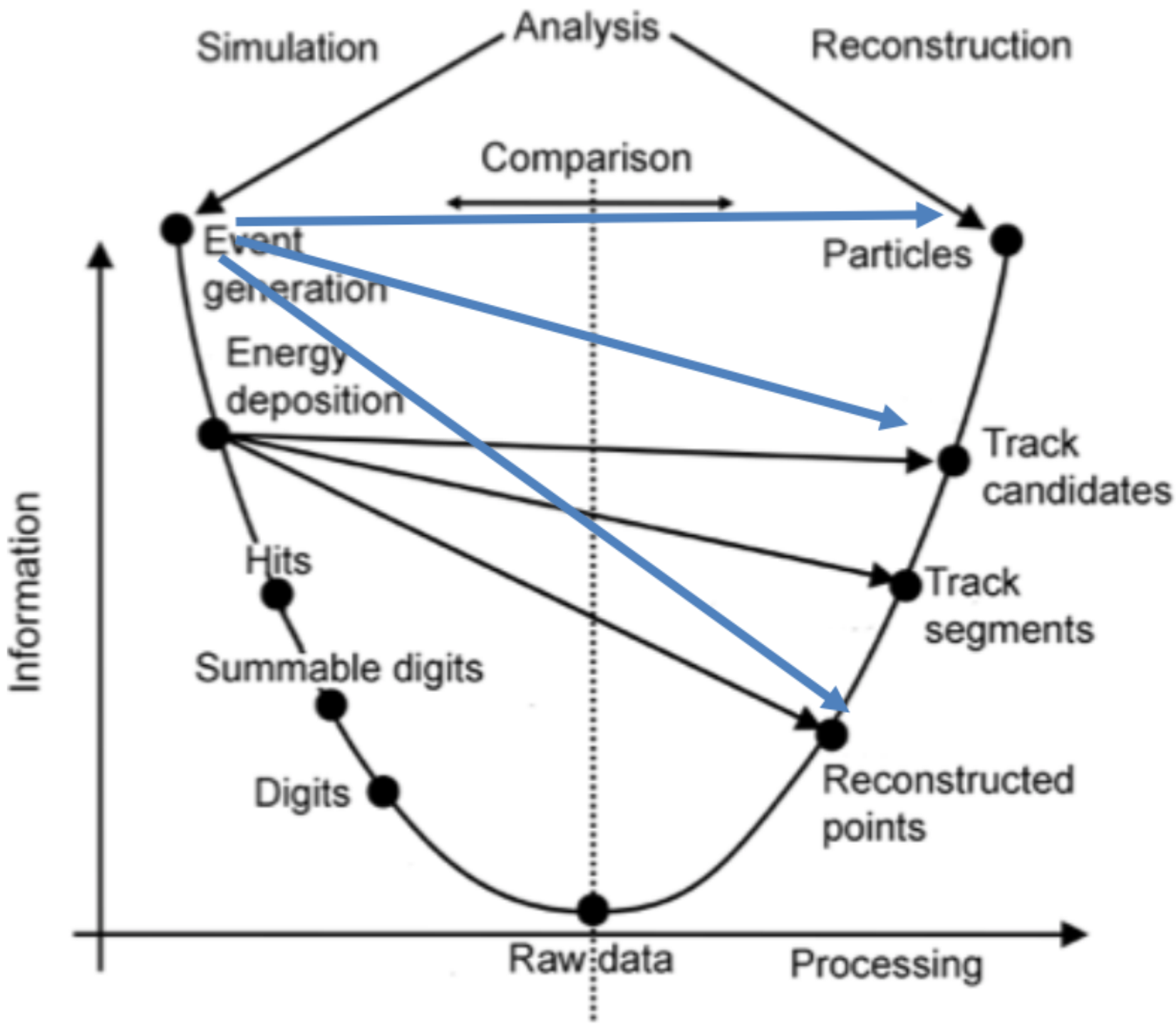
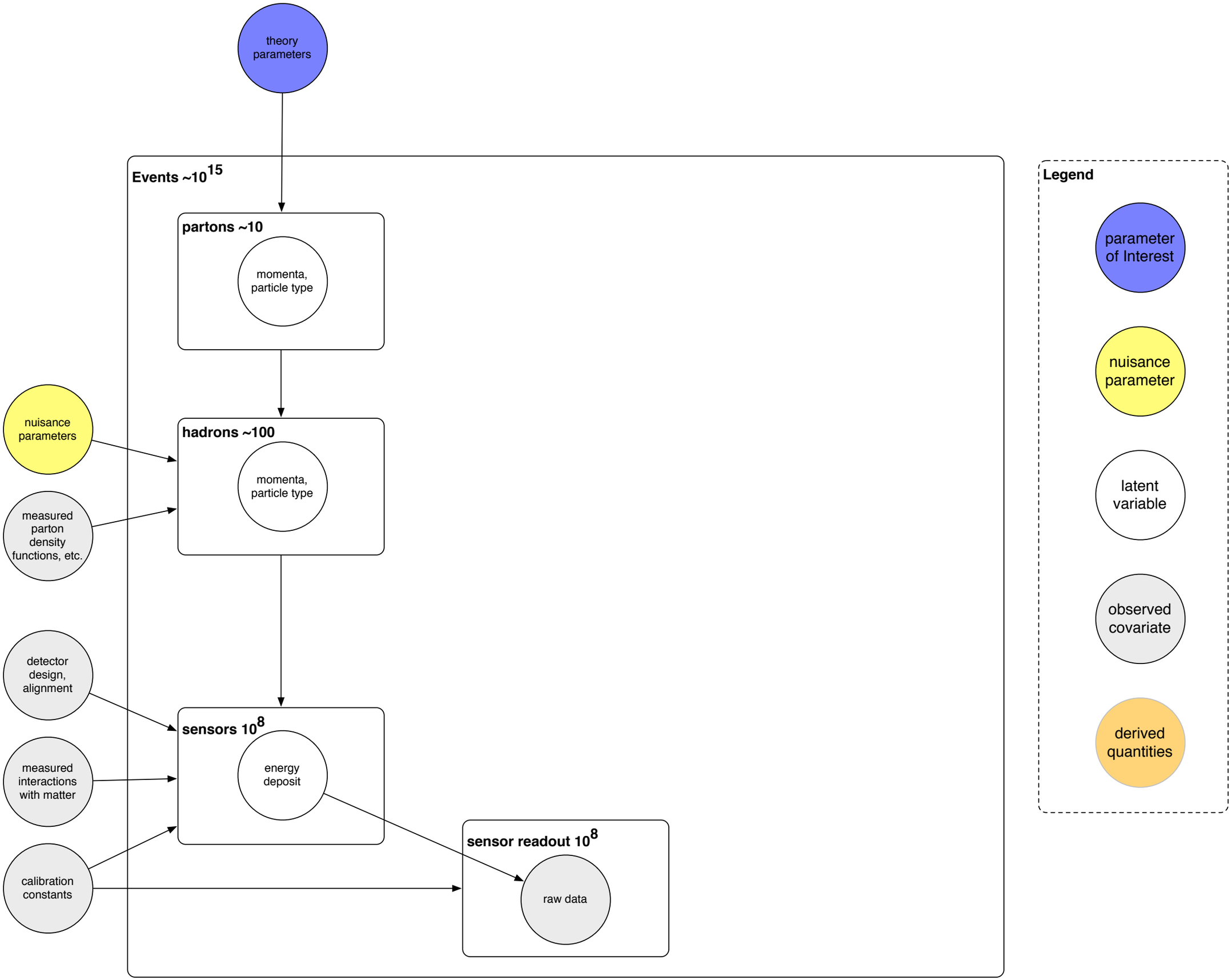
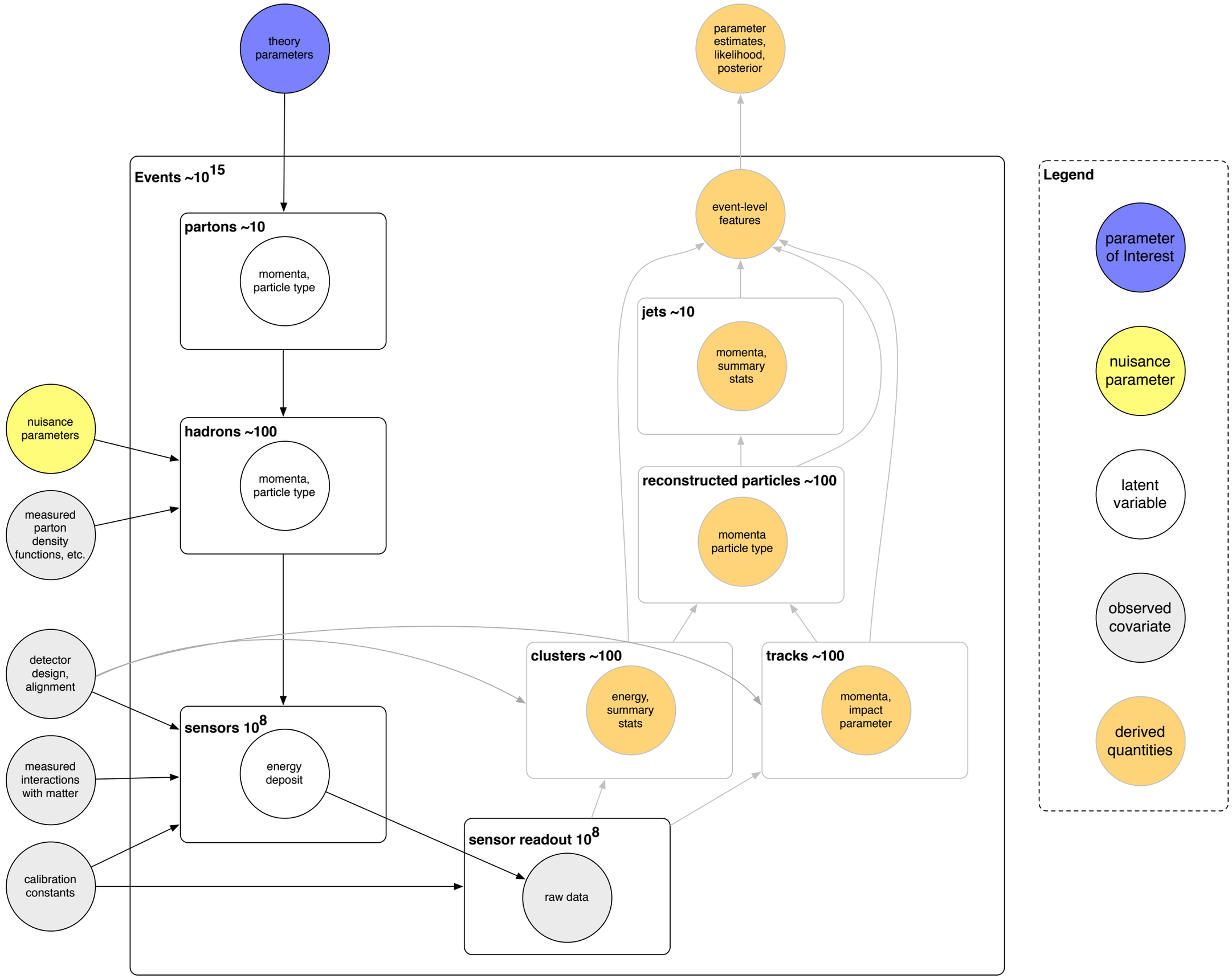


Figure by Federico Carminati, independent parallel inventions by Vincenzo Innocente & K.C.

FULL SIMULATION



FULL SIMULATION + RECONSTRUCTION



ML2.0?

How do these fit together?

Combine many of these ideas:

Large model, but **sparsely activated**

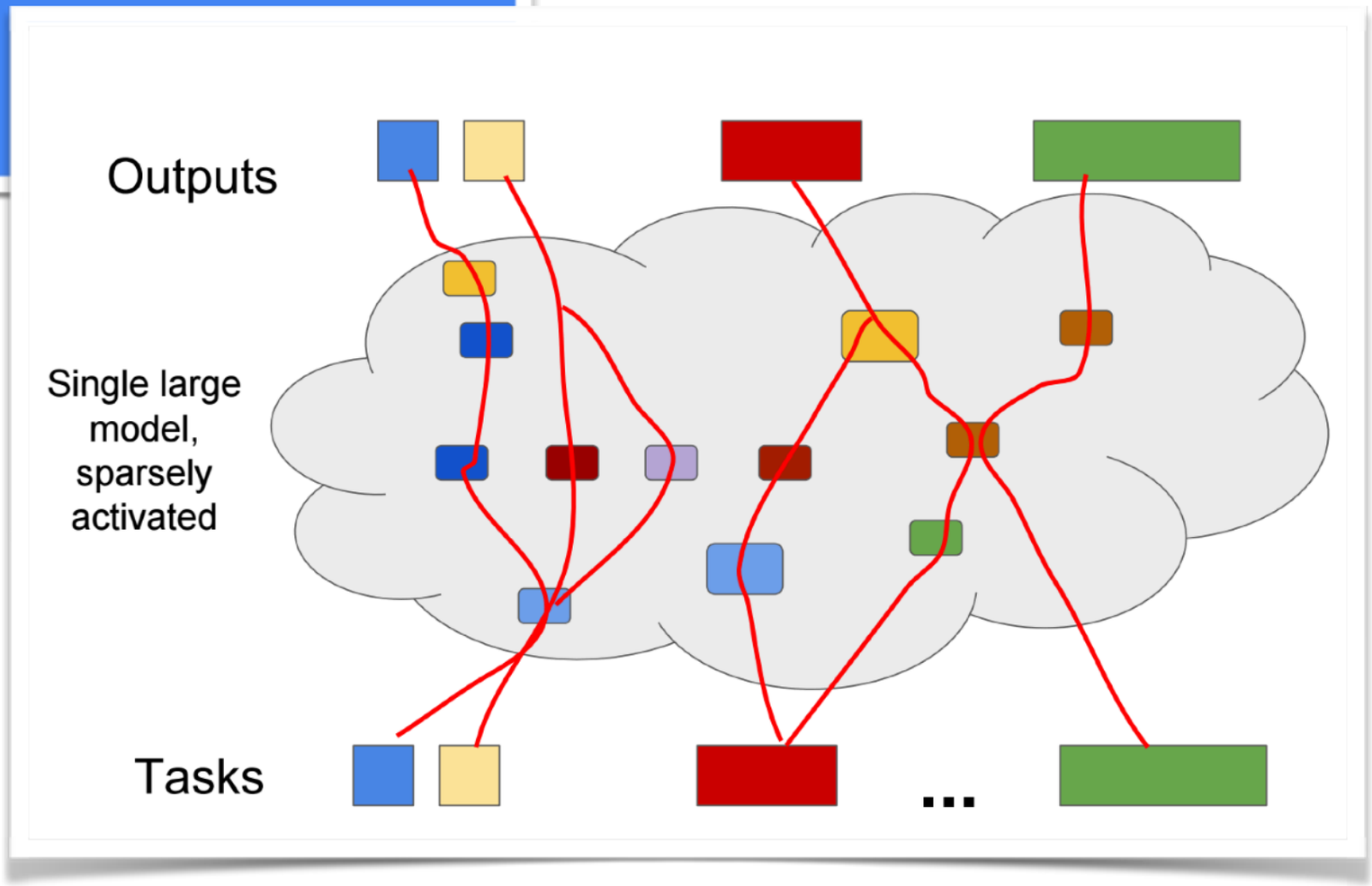
Single model to **solve many tasks** (100s to 1Ms)

Dynamically learn and **grow pathways** through large model

Hardware **specialized for ML supercomputing**

ML for efficient mapping onto this hardware

Google



Slides from Jeff Dean of Google Brain @ Jeju July 2017

https://drive.google.com/file/d/0B8z5oUpB2DysZWF1RTFuX1NEZUk/view

WHAT IS THE OBJECTIVE?

ML: What is the problem you are trying to solve?

Physicist: [eventually describes problem and formalizes objective]

ML: Ok, well let's optimize this directly …

Physicist: but, I also want….

Used to criticize physicists for constantly changing problem statement, but traditional approach to physics problems has many advantages

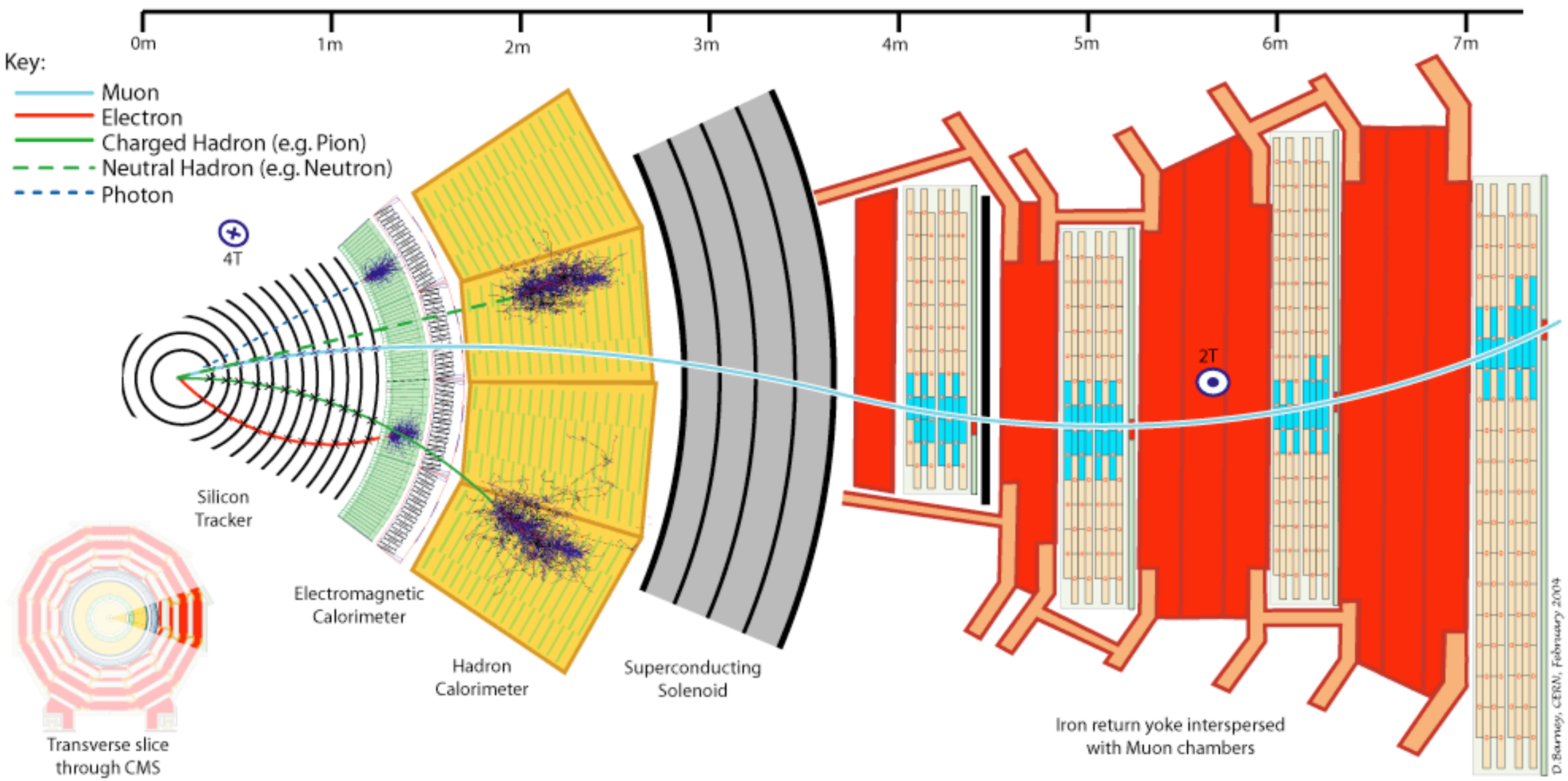
- modular, reusable components (facilitates transfer learning, "ML2.0")
- interpretable & individually validated
- a form of structural regularization

DETECTOR SIMULATION

Conceptually: Prob(detector response | particles)

Implementation: Monte Carlo integration over micro-physics

Consequence: evaluation of the likelihood is intractable



DETECTOR SIMULATION

Conceptually: Prob(detector response | particles)

Implementation: Monte Carlo integration over micro-physics

Consequence: evaluation of the likelihood is intractable

This motivates a new class of algorithms for what is called **likelihood-free inference**, which only require ability to generate samples from the simulation in the "forward mode"

A COMMON THEME

ABC

resources on approximate Bayesian computational methods

Search

Home

Home

This website keeps track of developments in approximate Bayesian computation (ABC) (a.k.a. likelihood-free), a class of computational statistical methods for Bayesian inference under intractable likelihoods. The site is meant to be a resource both for biologists and statisticians who want to learn more about ABC and related methods. Recent publications are under Publications 2012. A comprehensive list of publications can be found under Literature. If you are unfamiliar with ABC methods see the Introduction. Navigate using the menu to learn more.

ABC in Montreal | ABC in Montreal (2014)

ABC in Montreal

Approximate Bayesian computation (ABC) or likelihood-free (LF) methods have developed mostly beyond the radar of the machine learning community, but are important tools for a large and diverse segment of the scientific community. This is particularly true for systems and population biology, computational neuroscience, computer vision, healthcare sciences, but also many others.

Interaction between the ABC and machine learning community has recently started and contributed to important advances. In general, however, there is still significant room for more intense interaction and collaboration. Our workshop aims at being a place for this to happen.

Likelihood-free inference with neural networks

Example: Higgs Effective Field Theory

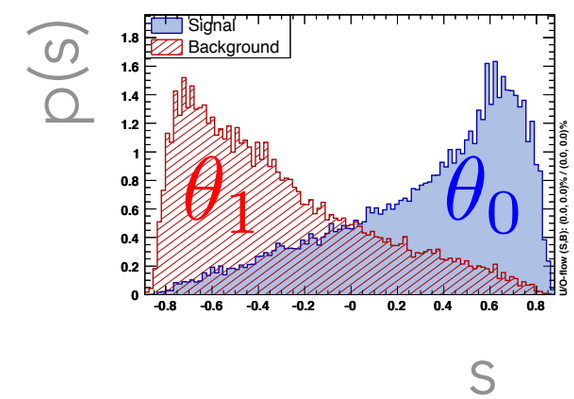
CARL

The intractable likelihood ratio based on high-dimensional features x is:

$$\frac{p(x|\theta_0)}{p(x|\theta_1)}$$

We can show that an **equivalent test** can be made from 1-D projection

$$\frac{p(x|\theta_0)}{p(x|\theta_1)} = \frac{p(s(x;\theta_0,\theta_1)|\theta_0)}{p(s(x;\theta_0,\theta_1)|\theta_1)}$$



if the scalar map s: X → $\mathbb{R}$ has the same level sets as the likelihood ratio

$$s(x;\theta_0;\theta_1) = \text{monotonic}[\ p(x|\theta_0)/p(x|\theta_1)\ ]$$

Estimating the density of $s(x;\theta_0,\theta_1)$ via the simulator calibrates the ratio.

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

CARL SOFTWARE

Gilles Louppe

http://diana-hep.org/carl/

diana-hep.org

DiscoveryLinks Higgs RooStats ALEPH Apple News Life Stuff ATLAS Wikipedia, inSpire Theory&Practice nyu espace JCSS HCG

Meet F Jupyter Note... Weekend rea... early-career-... 2016 Electio... 12-day Event... Joint meetin... carl API

Fork me on GitHub

Index

Sub-modules

- carl.data
- carl.distributions
- carl.learning
- carl.ratios

Notebooks

- Composing and fitting distributions
- Diagnostics for approximate likelihood ratios
- Likelihood ratios of mixtures of normals
- Parameterized inference from multidimensional data
- Parameterized inference with nuisance parameters

Display a menu

carl module

`carl` is a toolbox for likelihood-free inference in Python.

The likelihood function is the central object that summarizes the information from an experiment needed for inference of model parameters. It is key to many areas of science that report the results of classical hypothesis tests or confidence intervals using the (generalized or profile) likelihood ratio as a test statistic. At the same time, with the advance of computing technology, it has become increasingly common that a simulator (or generative model) is used to describe complex processes that tie parameters of an underlying theory and measurement apparatus to high-dimensional observations. However, directly evaluating the likelihood function in these cases is often impossible or is computationally impractical.

In this context, the goal of this package is to provide tools for the likelihood-free setup, including likelihood (or density) ratio estimation algorithms, along with helpers to carry out inference on top of these.

This project is still in its early stage of development. Join us on GitHub if you feel like contributing!

build passing | coverage 91% | DOI 10.5281/zenodo.47798

Likelihood-free inference with calibrated classifiers

Extensive details regarding likelihood-free inference with calibrated classifiers can be found in the companion paper *"Approximating Likelihood Ratios with Calibrated Discriminative Classifiers", Kyle Cranmer, Juan Pavez, Gilles Louppe.* http://arxiv.org/abs/1506.02169

Installation

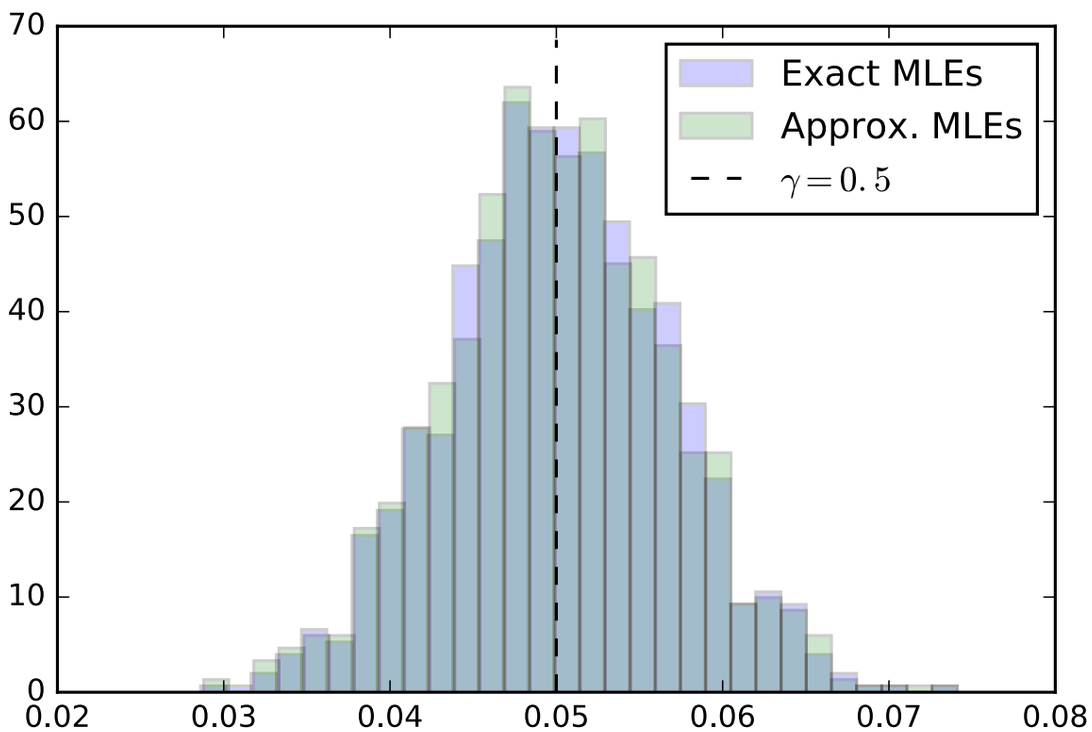
The following dependencies are required:

- Numpy >= 1.11

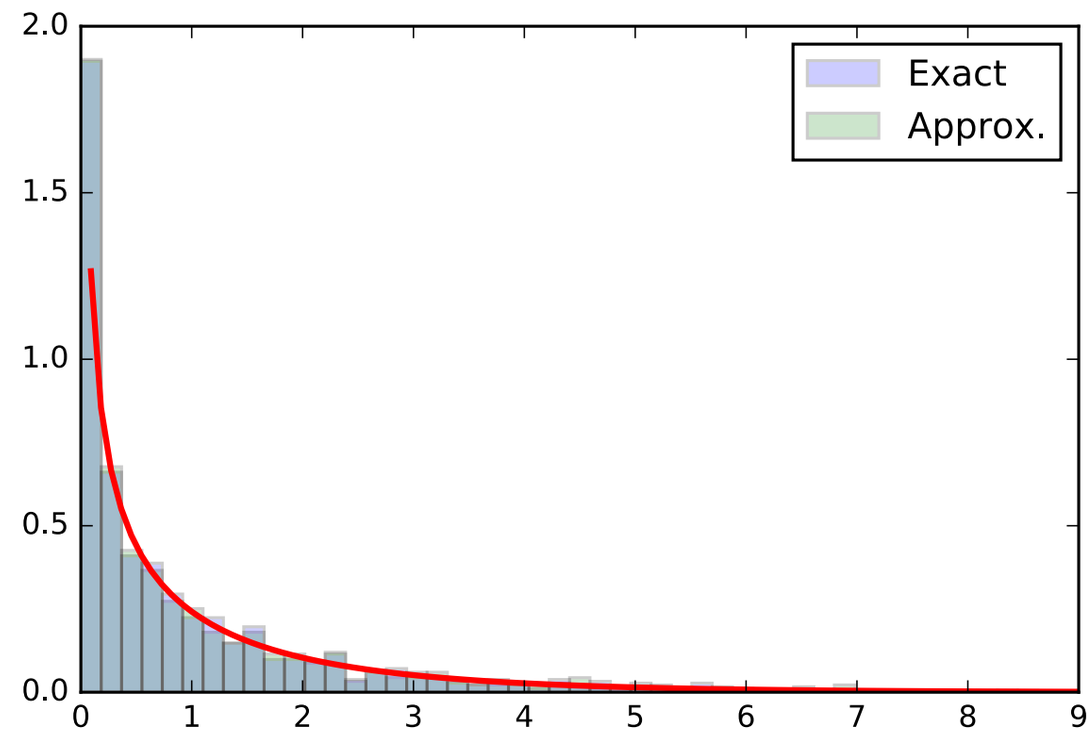
AMORTIZED LIKELIHOOD-FREE INFERENCE

Once we've learned the function s(x; θ) to approximate the likelihood, we can apply it to any data x.

- Here we check asymptotic distribution of profile likelihood ratio (Wilks's theorem)



(a) Exact vs. approximated MLEs.

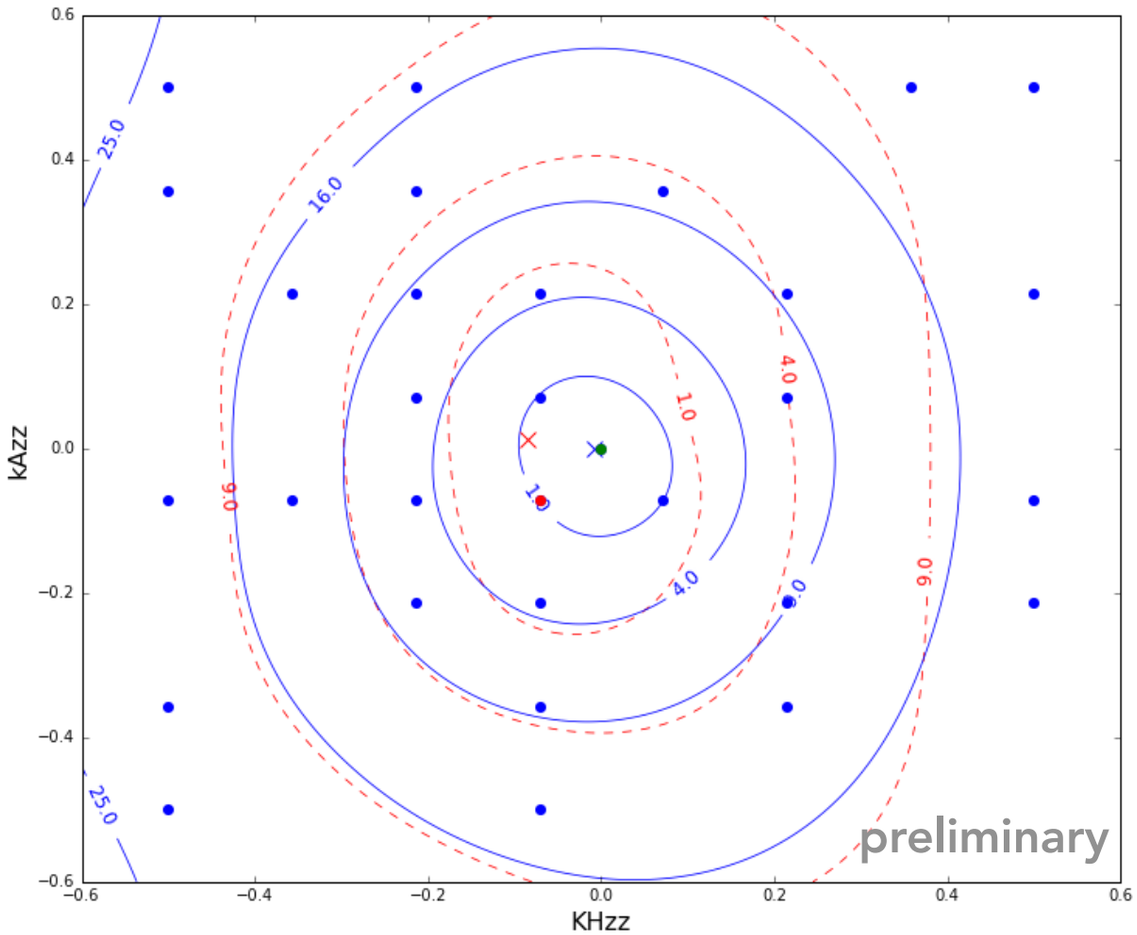


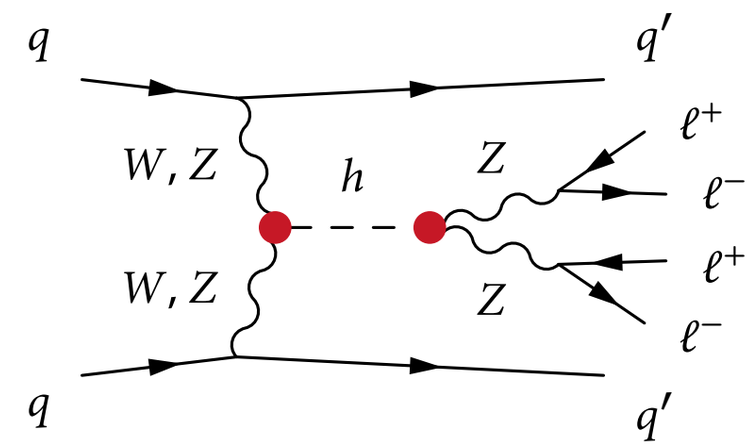
(b) $p(-2\log\Lambda(\gamma = 0.05)\,|\,\gamma = 0.05)$

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

APPLICATION TO THE HIGGS

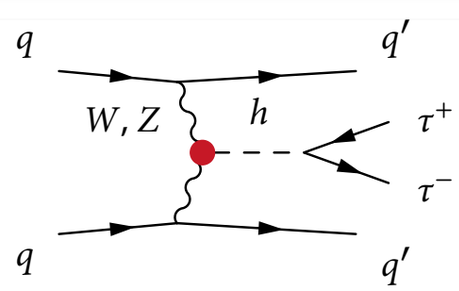
Preliminary work using fast detector simulation and CARL to approximate likelihoods using full kinematic information parametrized in 5-d coefficients of a Quantum Field Theory





16 observables
(using the CARL)

2 observables
(histogram templates)

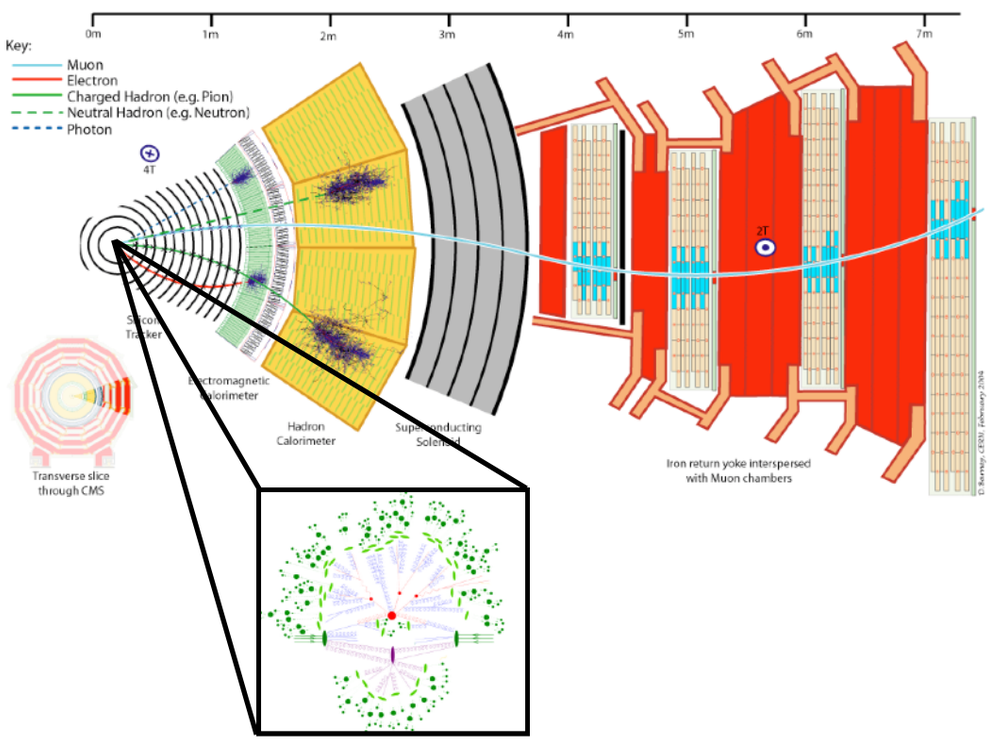


Equivalent to 3x more data.
(idealized, no systematic uncertainty)

work with Juan Pavez, Gilles Louppe, Cyril Becot, and Lukas Heinrich; Johann Brehmer, Felix Kling, and Tilman Plehn
"Better Higgs Measurements Through Information Geometry" [arXiv:1612.05261]

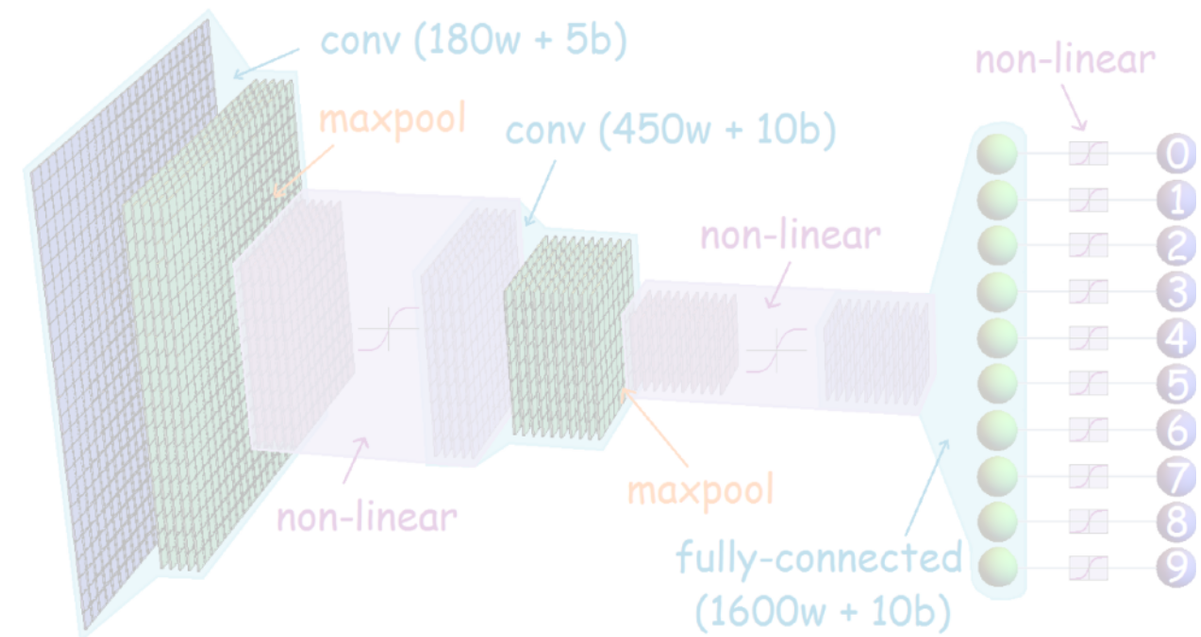
TWO APPROACHES

Use simulator
(much more efficiently)



- Approximate Bayesian Computation (ABC)
- Probabilistic Programming
- Adversarial Variational Optimization (AVO)

Learn simulator
(with deep learning)



- Generative Adversarial Networks (GANs), Variational Auto-Encoders (VAE)
- Likelihood ratio from classifiers (CARL)
- Autogregressive models, Normalizing Flows

[image credit: A.P. Goucher]

NEW! AVO

G. Louppe & K.C. arXiv:1707.07113

Adversarial Variational Optimization of Non-Differentiable Simulators

Gilles Louppe[1] and **Kyle Cranmer**[1]
[1]*New York University*

Complex computer simulators are increasingly used across fields of science as generative models tying parameters of an underlying theory to experimental observations. Inference in this setup is often difficult, as simulators rarely admit a tractable density or likelihood function. We introduce Adversarial Variational Optimization (AVO), a likelihood-free inference algorithm for fitting a non-differentiable generative model incorporating ideas from empirical Bayes and variational inference. We adapt the training procedure of generative adversarial networks by replacing the differentiable generative network with a domain-specific simulator. We solve the resulting non-differentiable minimax problem by minimizing variational upper bounds of the two adversarial objectives. Effectively, the procedure results in learning a proposal distribution over simulator parameters, such that the corresponding marginal distribution of the generated data matches the observations. We present results of the method with simulators producing both discrete and continuous data.

Leo is G Tom is D

Similar to GAN setup, but instead of using a neural network as the generator, use the actual simulation (eg. Pythia, GEANT)

Continue to use a neural network discriminator / critic.

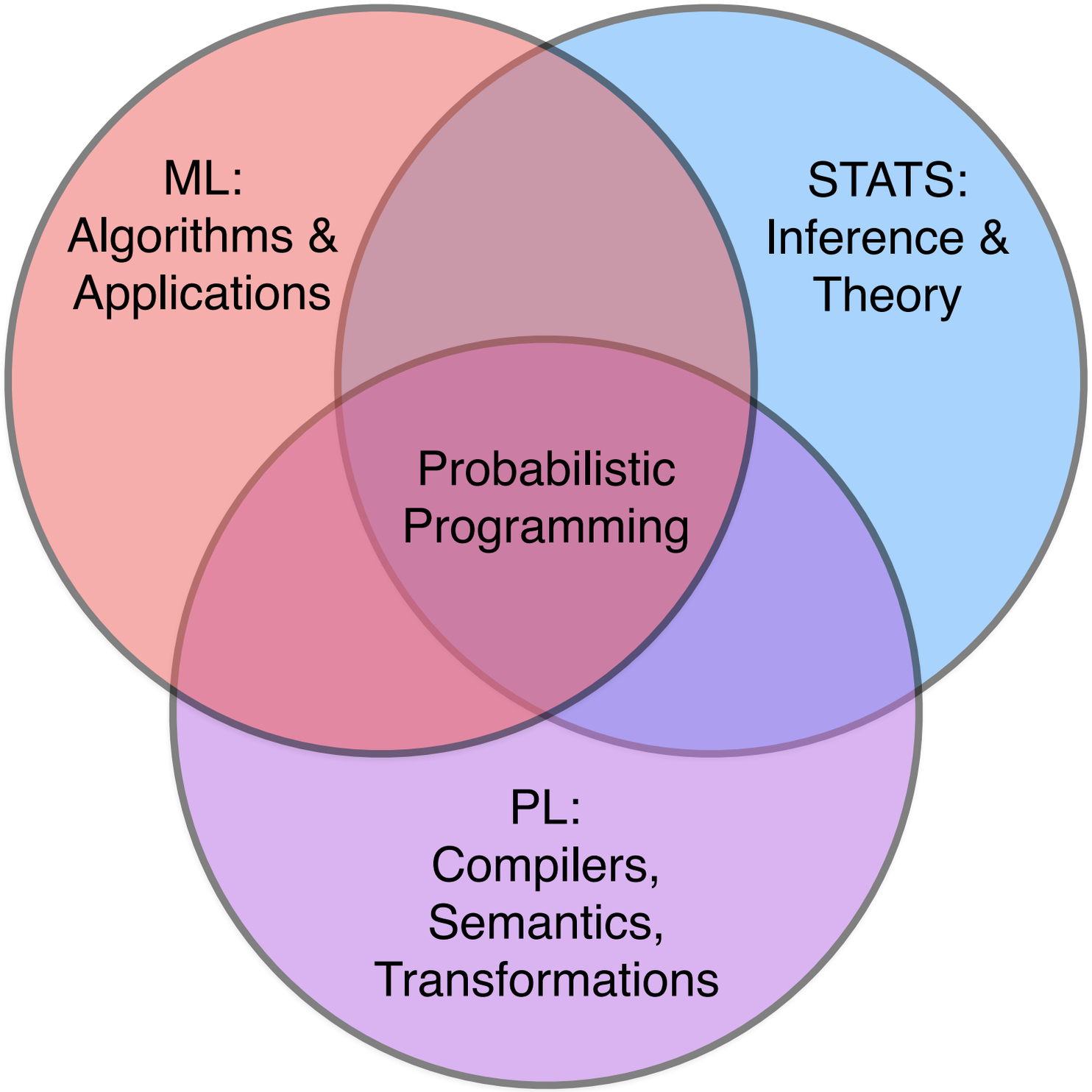
Difficulty: the simulator isn't differentiable, but there's a **trick**!

Allows us to efficiently fit / **tune simulation** with stochastic gradient techniques!

Probabilistic Programming: Inverting the simulation

(very ambitious)

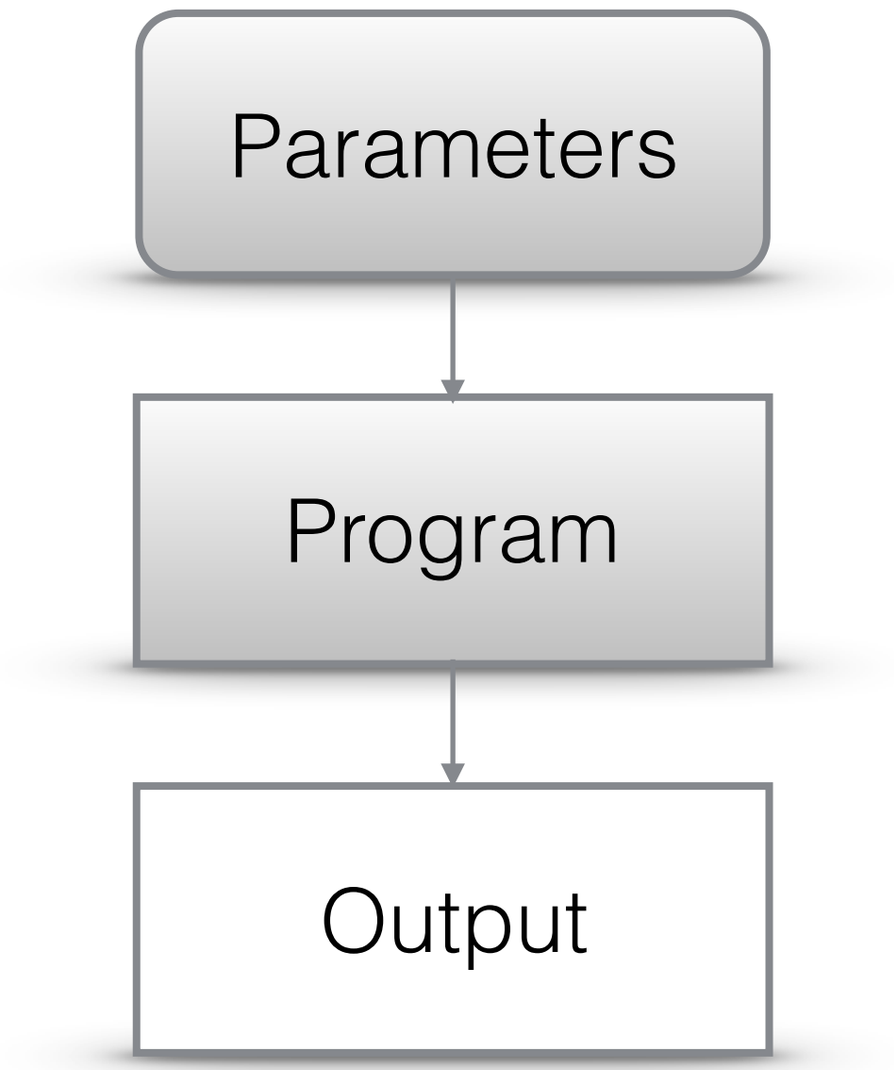
Probabilistic Programming



Intuition

[slides, Frank Wood]

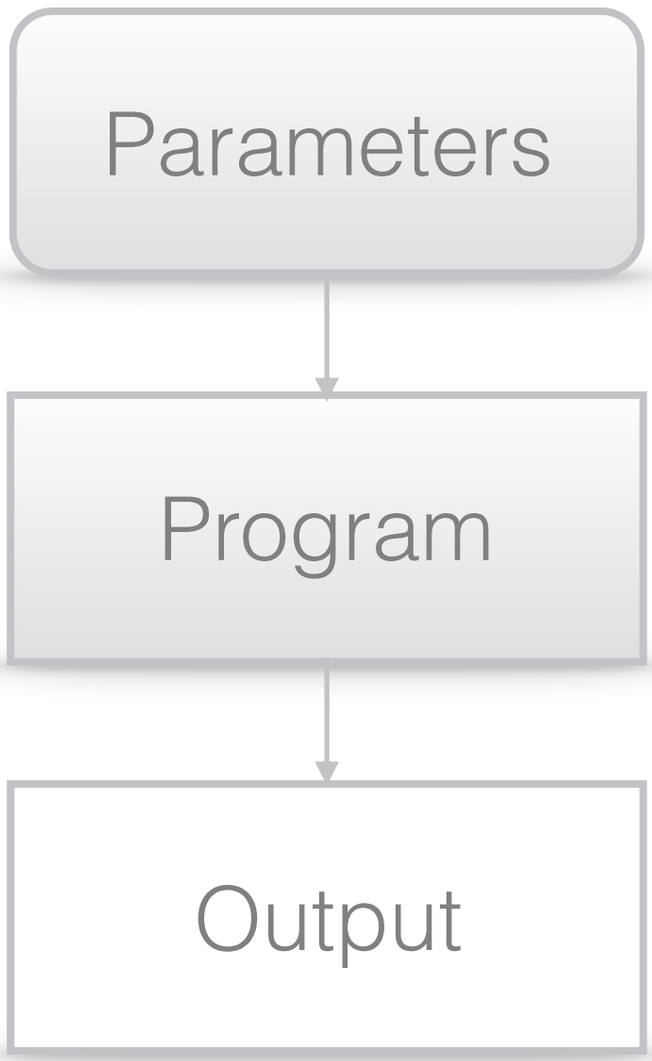
Intuition



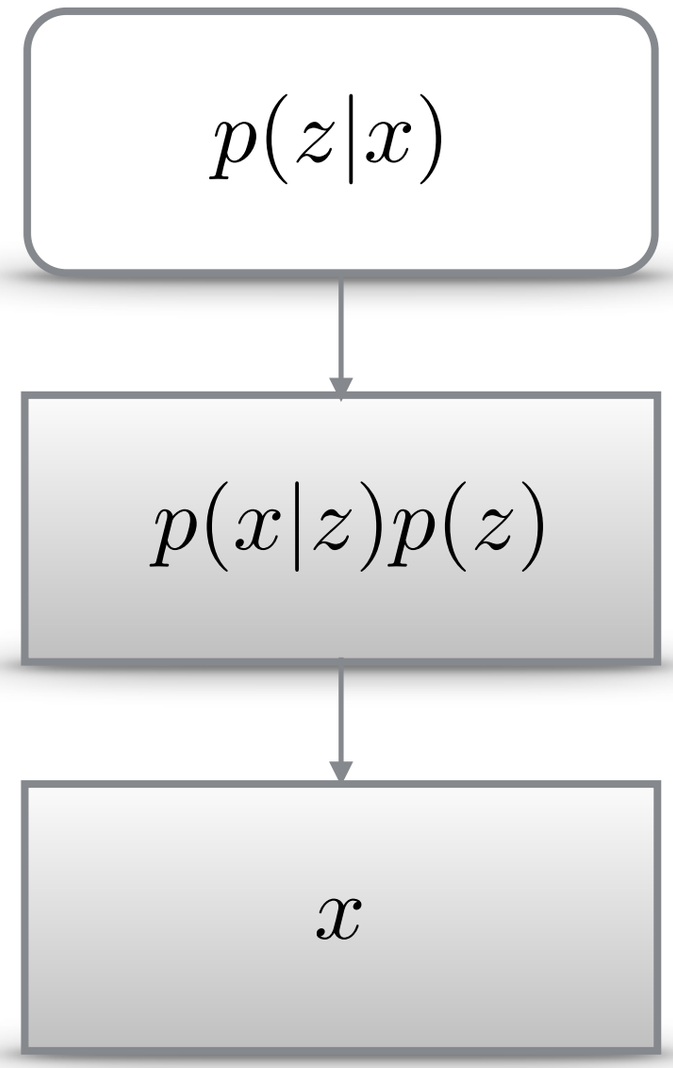
CS

[slides, Frank Wood]

Intuition



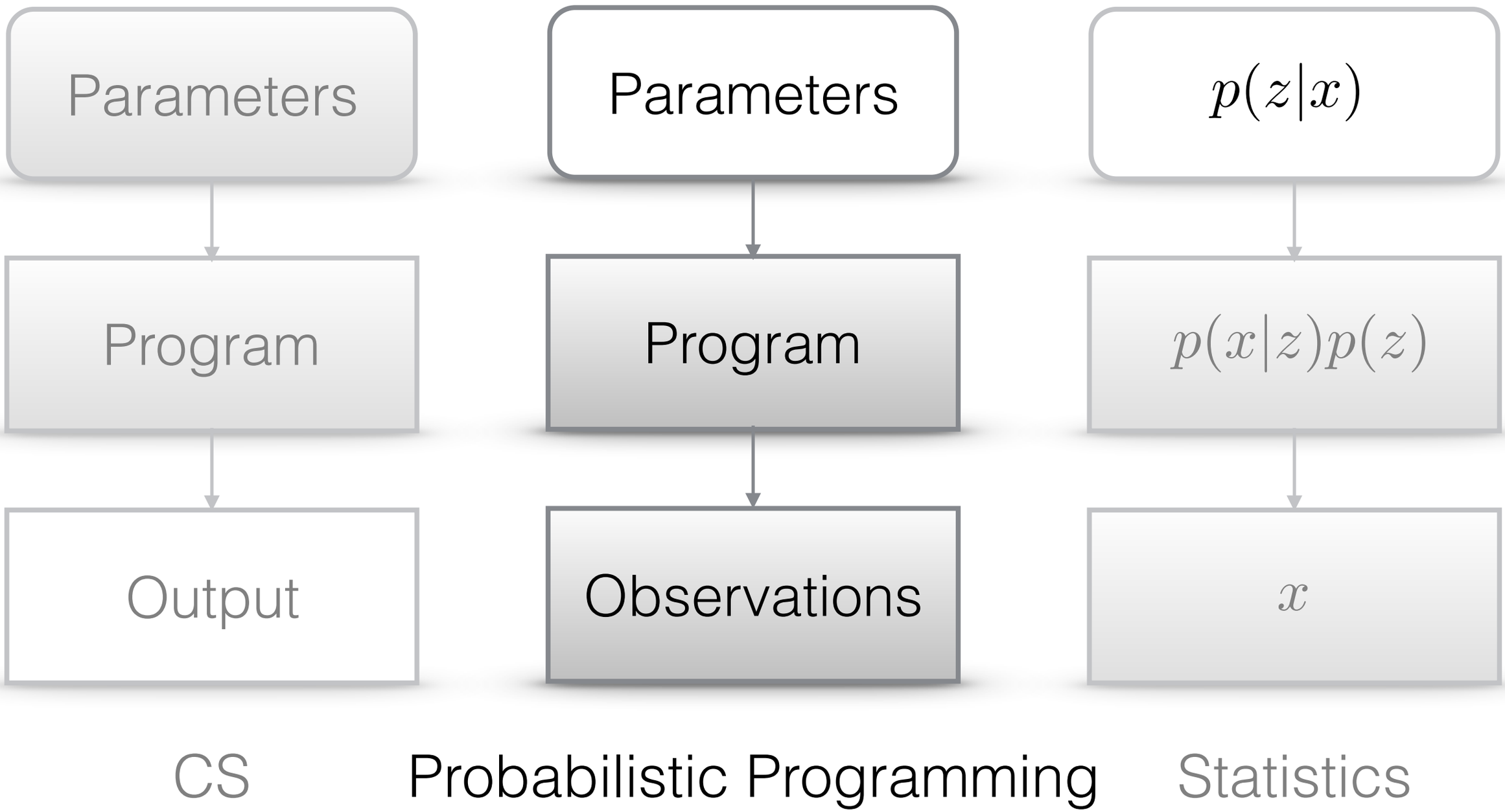
CS



Statistics

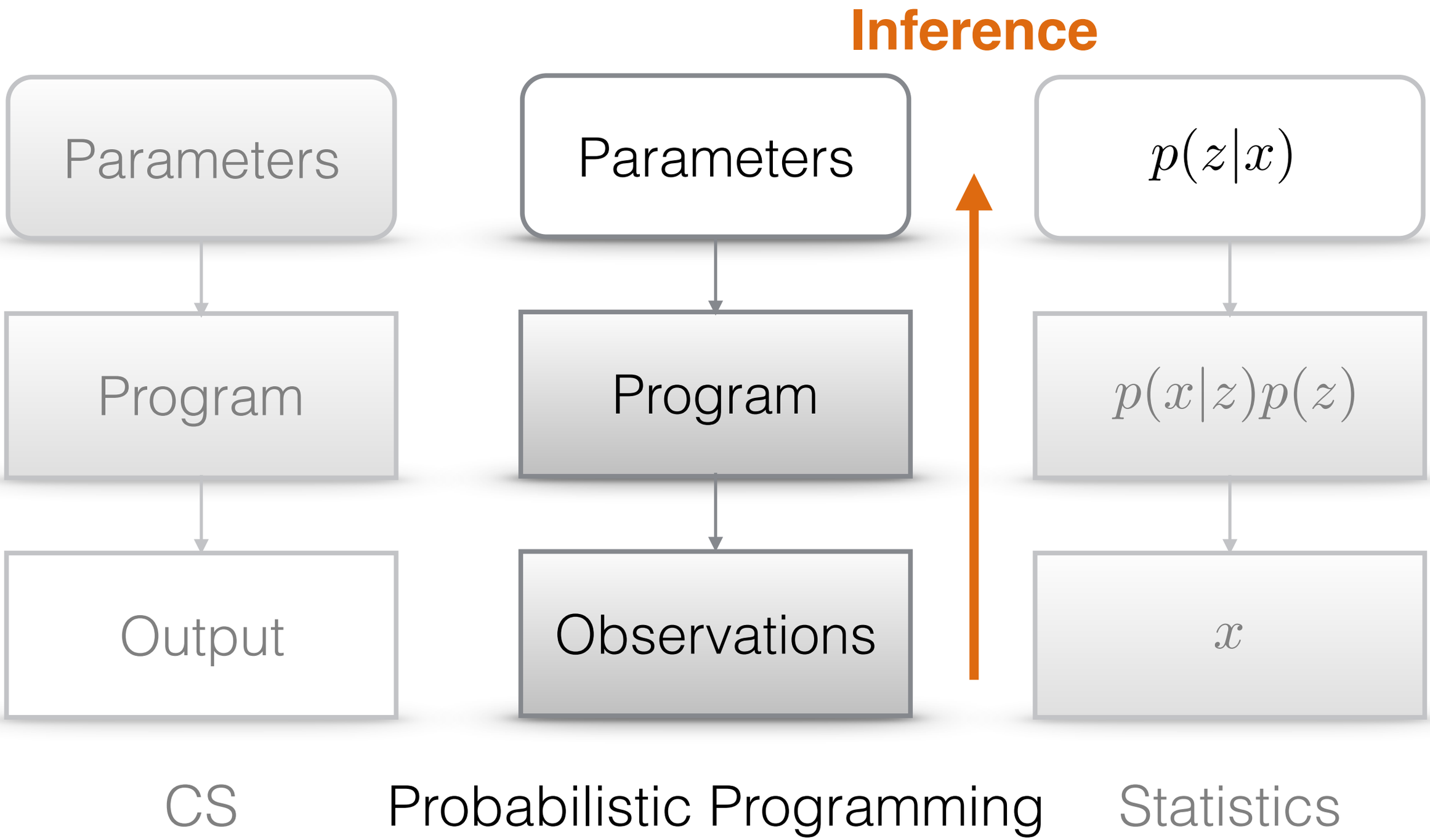
[slides, Frank Wood]

Intuition



[slides, Frank Wood]

Intuition



[slides, Frank Wood]

CAPTCHA breaking

Observation

Posterior Samples

Generative Model

```
(defquery captcha
 [image num-chars tol]
 (let [[w h] (size image)
       ;; sample random characters
       num-chars (sample
                  (poisson num-chars))
       chars (repeatedly
              num-chars sample-char)]
  ;; compare rendering to true image
  (map (fn [y z]
         (observe (normal z tol) y))
       (reduce-dim image)
       (reduce-dim (render chars w h)))
 ;; predict captcha text
 {:text
  (map :symbol (sort-by :x chars))}))
```

$\mathbf{x}$	$\mathbf{y}$
text	image

Mansinghka,, Kulkarni, Perov, and Tenenbaum
"Approximate Bayesian image interpretation using generative probabilistic graphics programs." NIPS (2013).

CAPTCHA breaking

Observation

Posterior Samples

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  ;; compare rendering to true image
  (map (fn [y z]
         (observe (normal z tol) y))
       (reduce-dim image)
       (reduce-dim (render chars w h)))
 ;; predict captcha text
 {:text
  (map :symbol (sort-by :x chars))}))
```

$\mathbf{x}$	$\mathbf{y}$
text	image

Mansinghka,, Kulkarni, Perov, and Tenenbaum
"Approximate Bayesian image interpretation using generative probabilistic graphics programs." NIPS (2013).

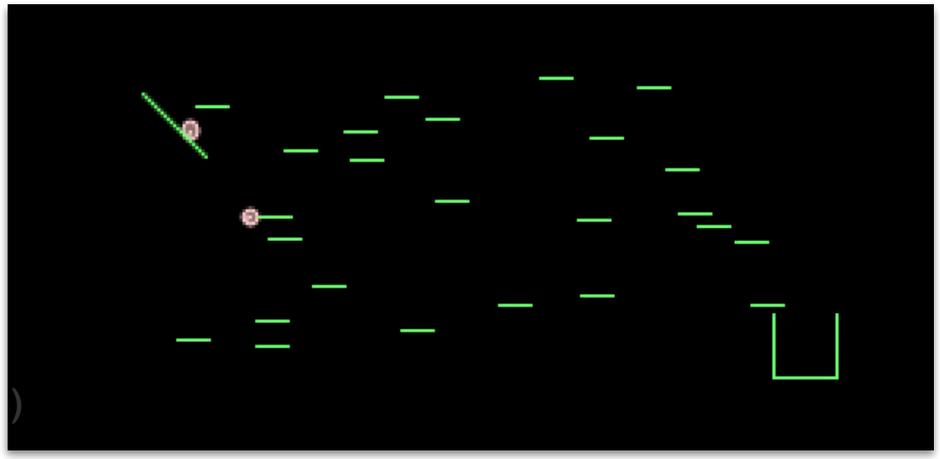
ANALOGY: RANDOM BUMPERS ~ RANDOM CALORIMETER SHOWER

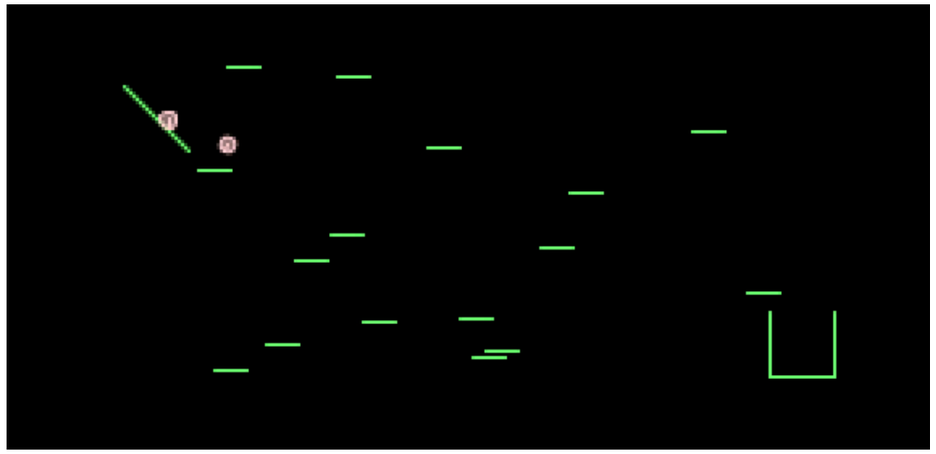
```
(defquery arrange-bumpers []
    (let [number-of-bumpers (sample (poisson 20))
          bumpydist (uniform-continuous 0 10)
          bumpxdist (uniform-continuous -5 14)
          bumper-positions (repeatedly
                            number-of-bumpers
                            #(vector (sample bumpxdist)
                                     (sample bumpydist)))

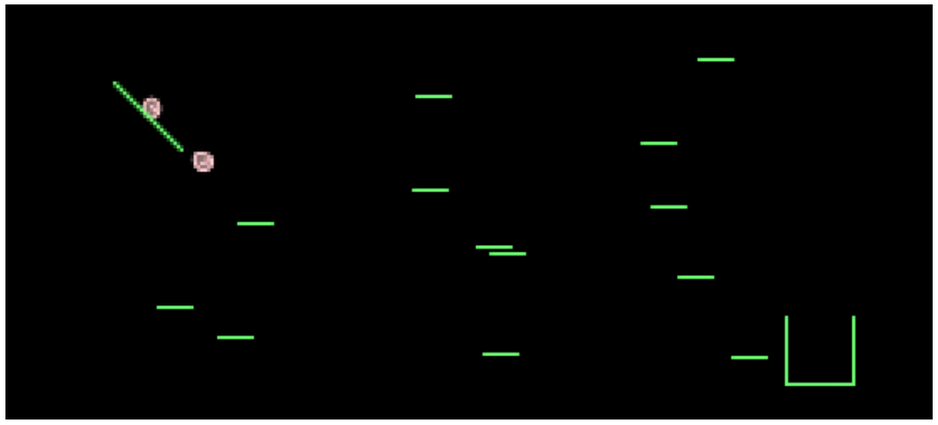
          ;; code to simulate the world
          world (create-world bumper-positions)
          end-world (simulate-world world)
          balls (:balls end-world)

          ;; how many balls entered the box?
          num-balls-in-box (balls-in-box end-world)]

      {:balls balls
       :num-balls-in-box num-balls-in-box
       :bumper-positions bumper-positions}))
```







3 examples generated from simulator

[slides, Frank Wood]

ANALOGY: RANDOM BUMPERS ~ RANDOM CALORIMETER SHOWER

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(defquery arrange-bumpers []
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       :num-balls-in-box num-balls-in-box
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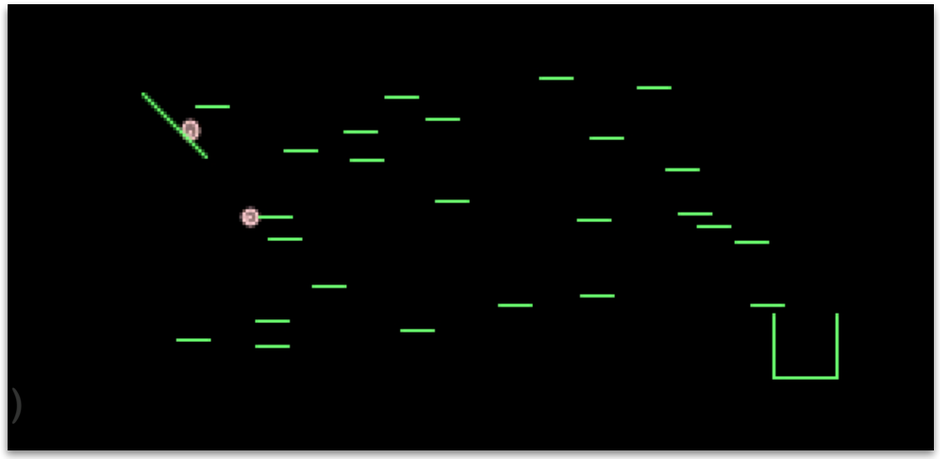

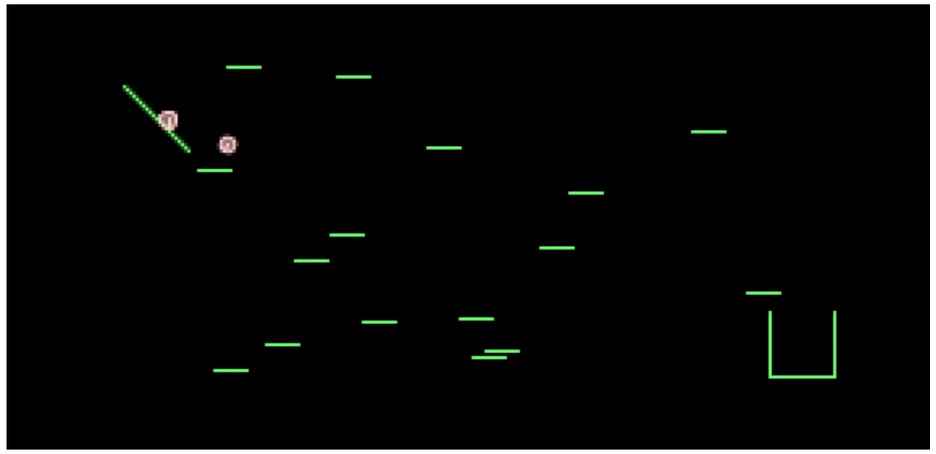

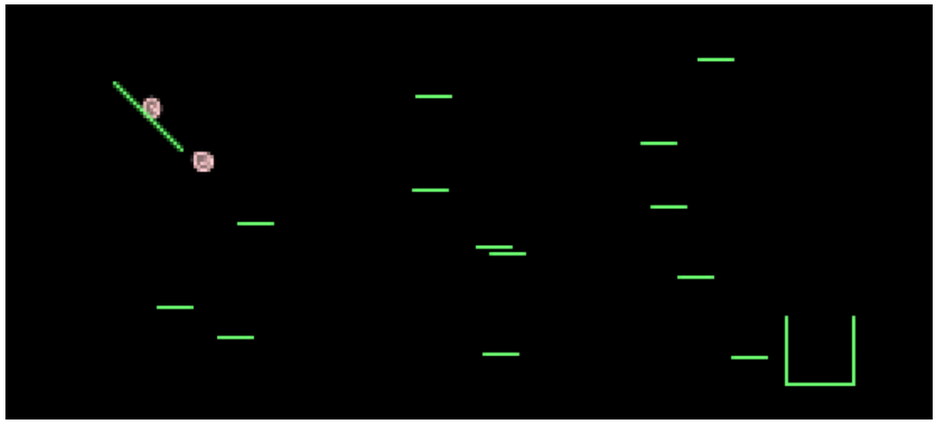

3 examples generated from simulator

[slides, Frank Wood]

UNDERSTANDING THE TAILS OF DISTRIBUTIONS

```
(defquery arrange-bumpers []
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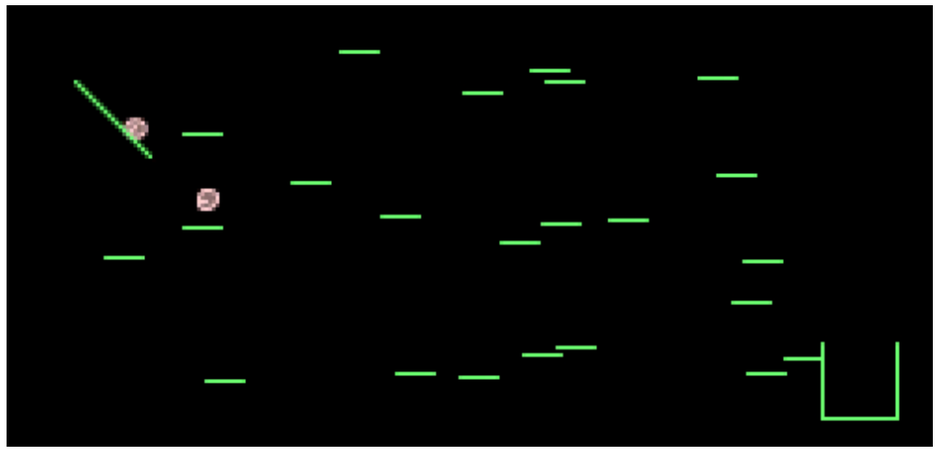
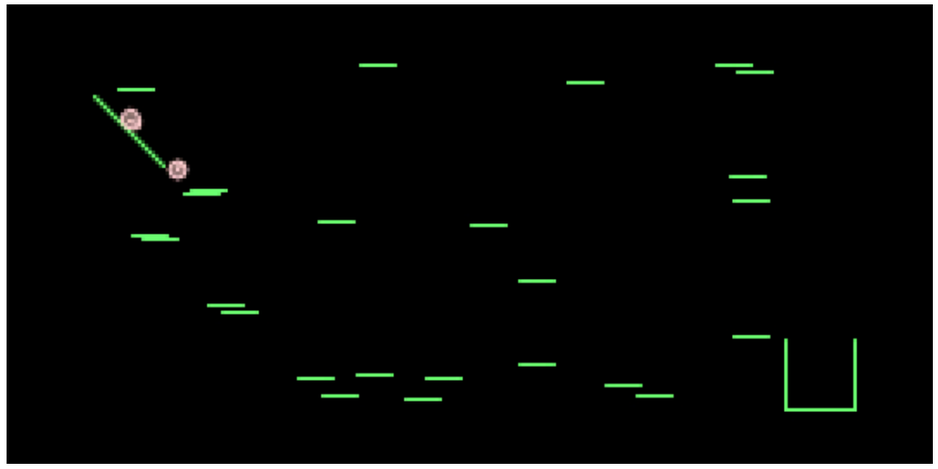
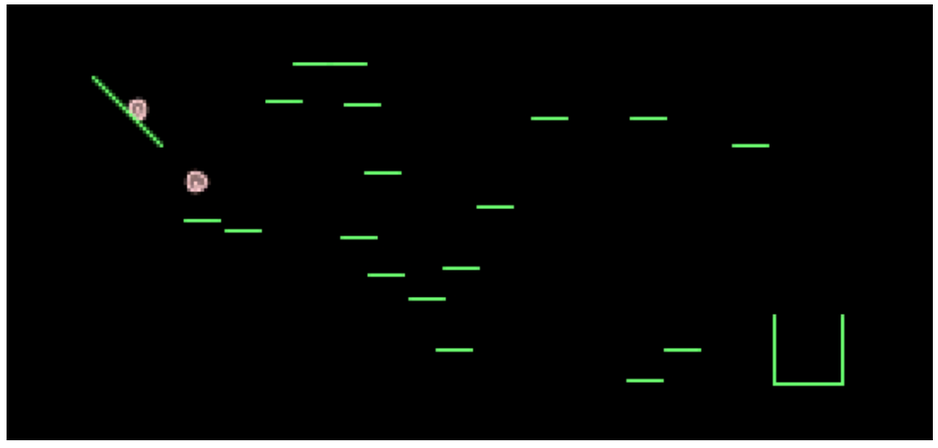
          num-balls-in-box (balls-in-box end-world)

          obs-dist (normal 4 0.1)]

    (observe obs-dist num-balls-in-box)
```







3 examples generated from simulator **conditioned** on ~20% of balls land in box (~ given observed energy deposits)

[slides, Frank Wood]

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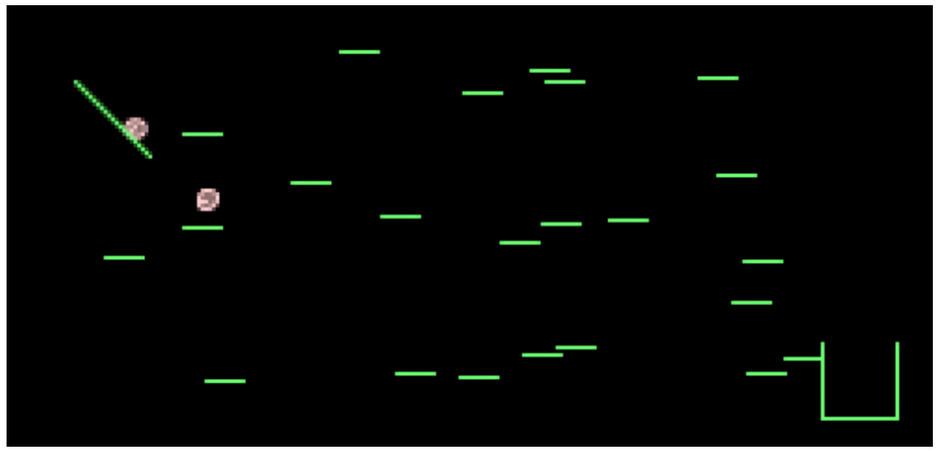
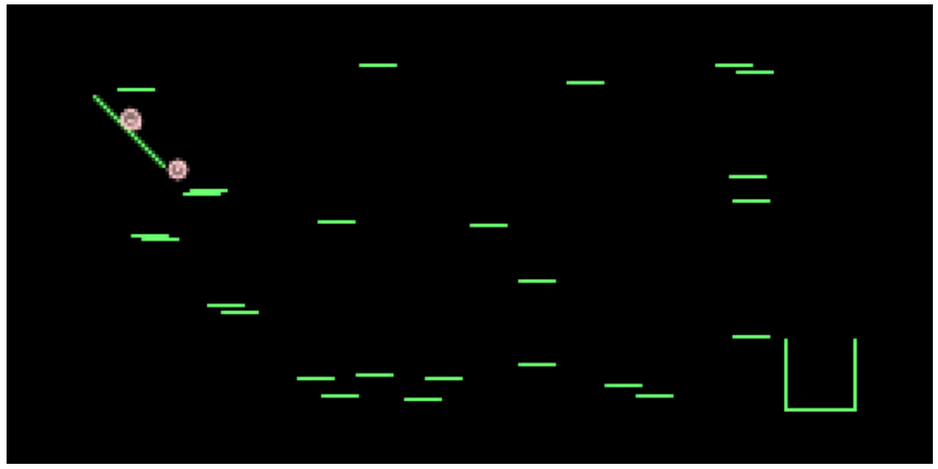
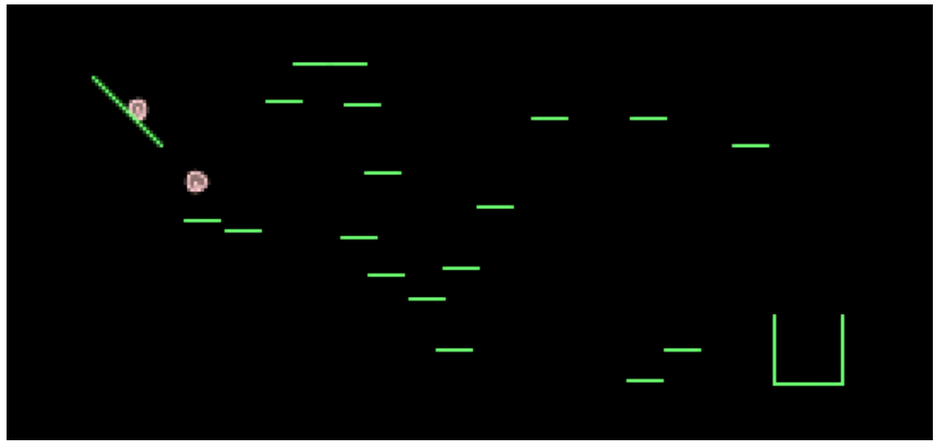






3 examples generated from simulator **conditioned** on ~20% of balls land in box (~ given observed energy deposits)

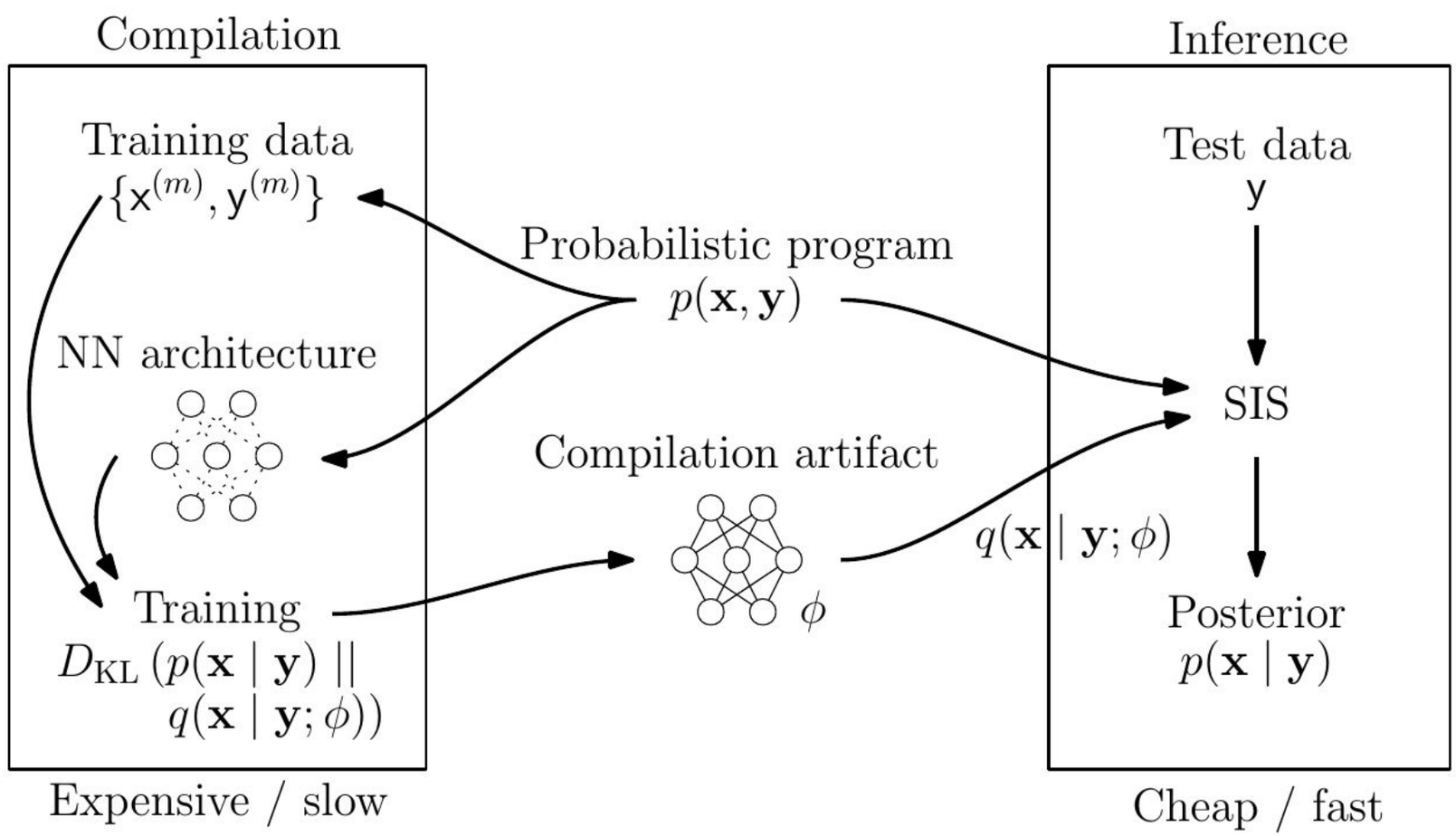
[slides, Frank Wood]

HOW DOES IT WORK?

In short: hijack the random number generators and use NN's to perform a *very* smart type of importance sampling

Input: an inference problem denoted in a universal PPL (Anglican, CPProb)

Output: a trained inference network, or "compilation artifact" (Torch, PyTorch)



Le, Baydin and Wood. Inference Compilation and Universal Probabilistic Programming. AISTATS 2017. *arXiv:1610.09900*

IN PROGRESS: C++, SHERPA, GEANT4

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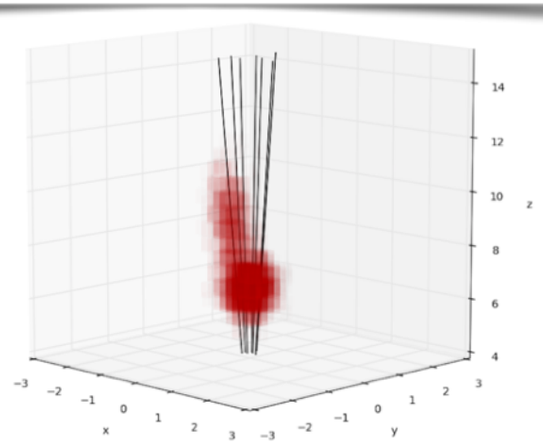


Probabilistic programming with C++

Our new tool: CPProb
https://github.com/probprog/cpprob

Instrumenting C++ code to allow tools like SHERPA and GEANT run with inference compilation

```
void linear_regression(const std::array<std::pair<RealType, RealType>, N> & points) {
    using boost::random::normal_distribution;

    auto normal = normal_distribution<RealType>{0, 10};
    const auto a = cpprob::sample(normal, true);
    const auto b = cpprob::sample(normal, true);

    for (const auto & point : points) {
        auto likelihood = normal_distribution<RealType>{a * point.first + b, 1};
        cpprob::observe(likelihood, point.second);
    }
    cpprob::predict(a);
    cpprob::predict(b);
}
```

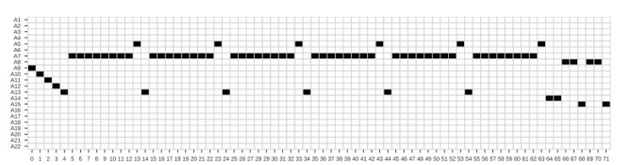
```
SHERPA::Hadron_Decays::Treat(ATOOLS::Blob_List*, double&)+0x709
SHERPA::Event_Handler::IterateEventPhases(SHERPA::eventtype::code&, double&)+0x1b2
SHERPA::Event_Handler::GenerateHadronDecayEvent(SHERPA::eventtype::code&)+0x979
```

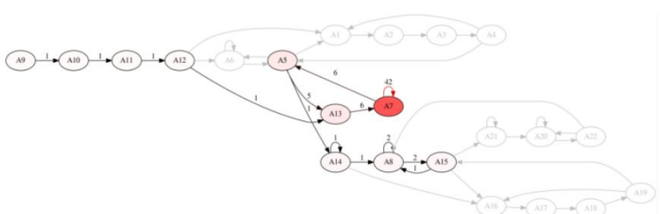
A case study in SHERPA & GEANT

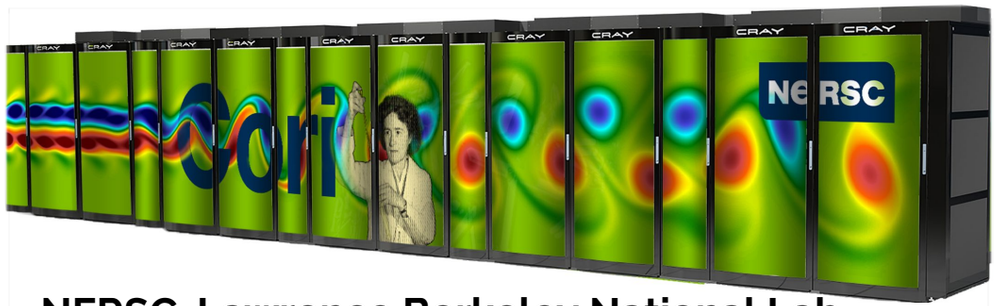
Probabilistic program analytics
allows us to **pinpoint "interesting" addresses** in execution traces
and corresponding **C++ code within SHERPA**

4.4.24 Unique trace T24

Length 72







NERSC, Lawrence Berkeley National Lab

Our current tools:
- CPProb
  - A new C++ PPL coupled with large-scale simulations using, e.g., SHERPA and GEANT
- PyTorch inference compilation backend
  - Dynamic computation graphs for NN artifacts

Designed to run on Cori at NERSC using Shifter

```
shifterimg -v pull docker:gbaydin/pytorch-infcomp:latest
shifterimg -v pull docker:gbaydin/sherpa-infcomp-full:latest
```

docker

Active Learning

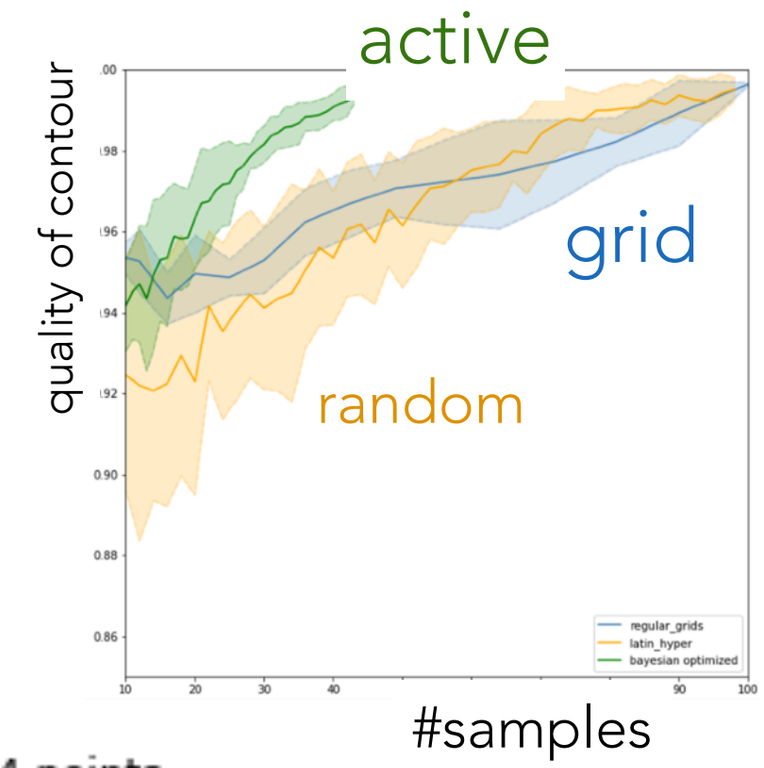
more efficient simulation

ACTIVE LEARNING

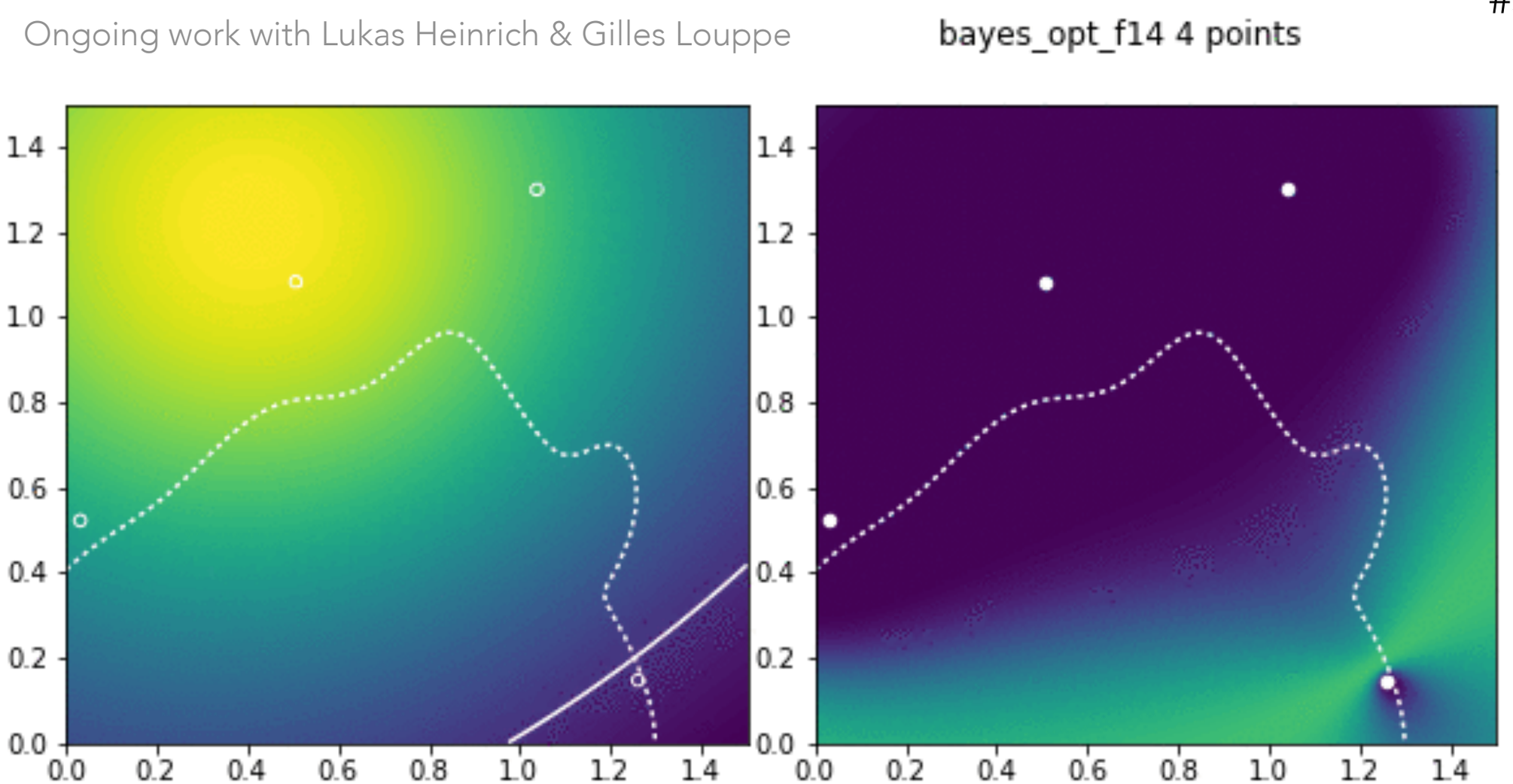
Instead of generating Monte Carlo a priori, generate it on demand where it is relevant!

↓ An algorithm for finding exclusion contours

Drastically more efficient use of computing resources →



Ongoing work with Lukas Heinrich & Gilles Louppe



ACTIVE LEARNING

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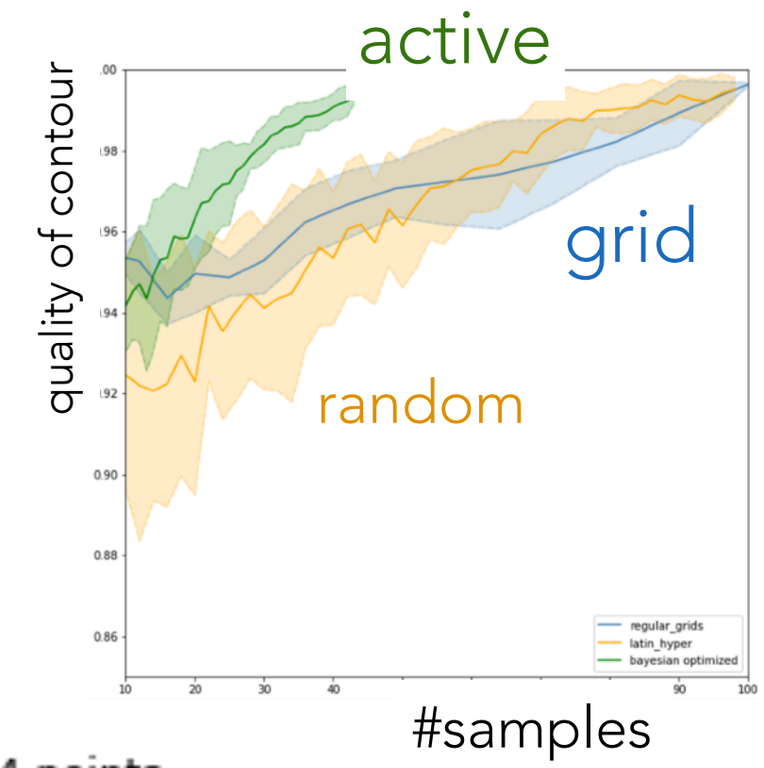

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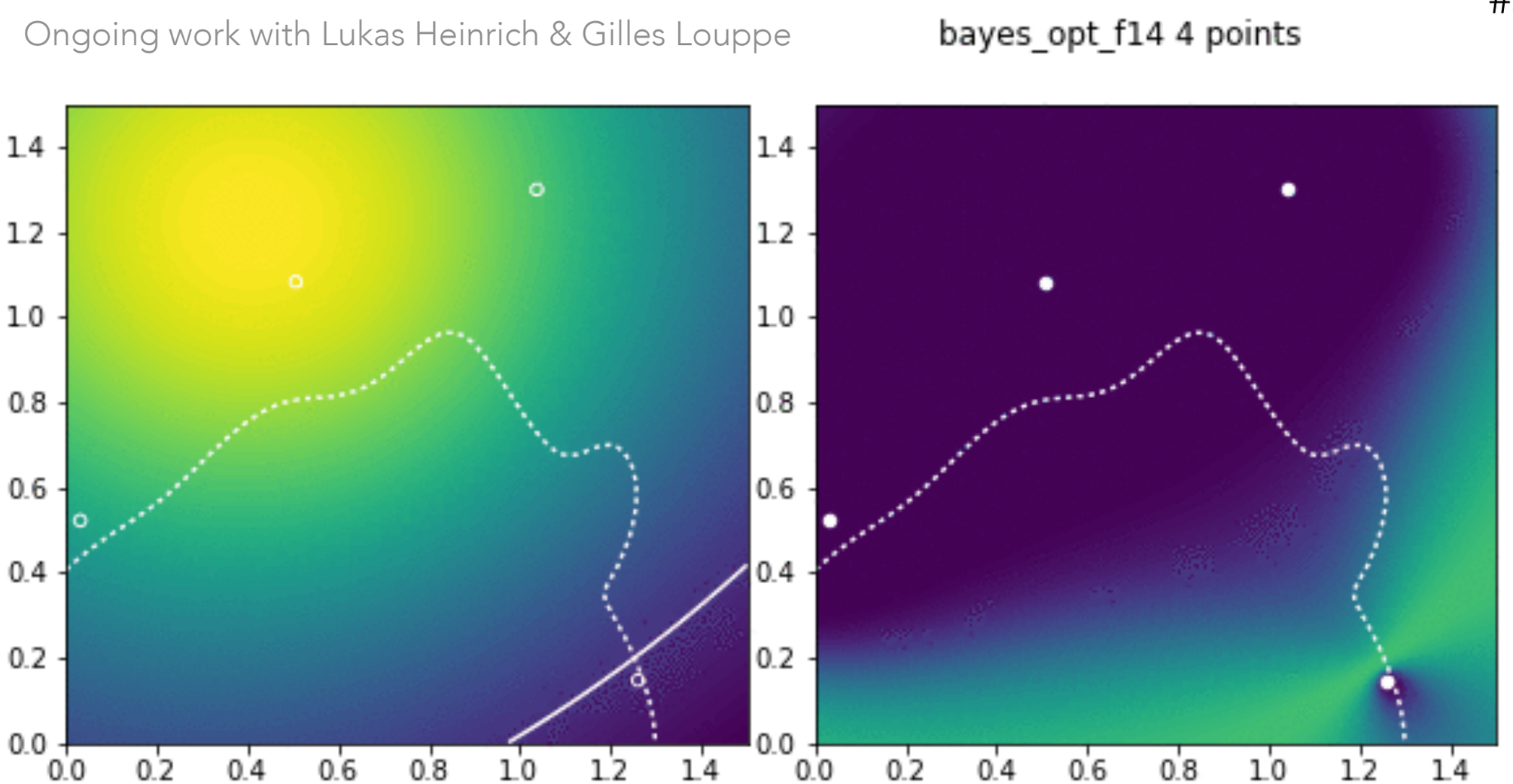


SYNTHESIS

active learning

Active Sciencing

reusable workflows

simulation-based
inference engines

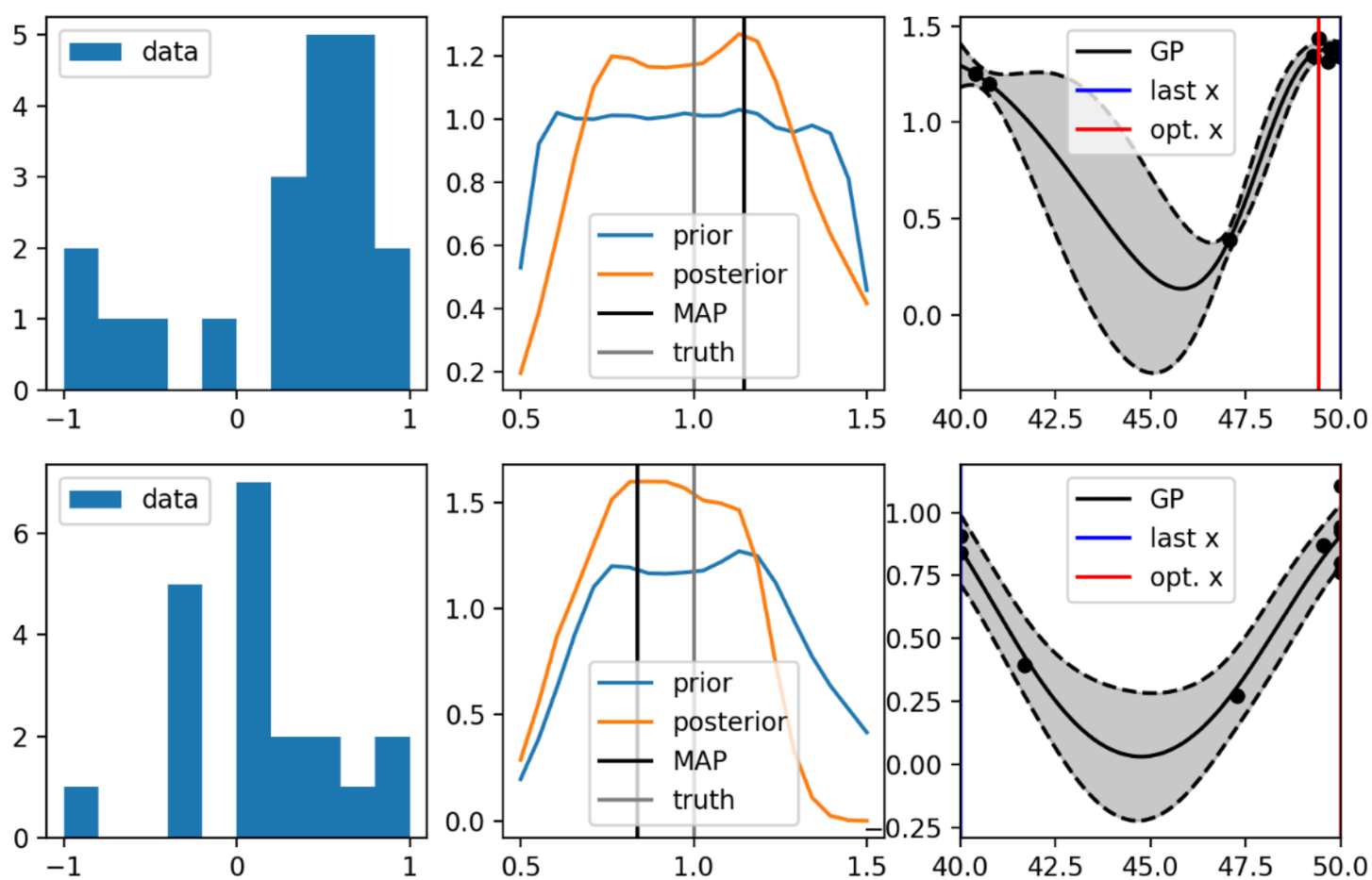
https://github.com/cranmer/active_sciencing

ACTIVE SCIENCING DEMO

Input:

- workflow for performing "real" experiment that returns data
- workflow for running simulator given parameters of theory and experimental configuration

Demo shows use of likelihood-free inference technique & Bayesian Optimization to measure the Weinberg angle and optimize beam energy (eg. just above or below $M_Z/2$)



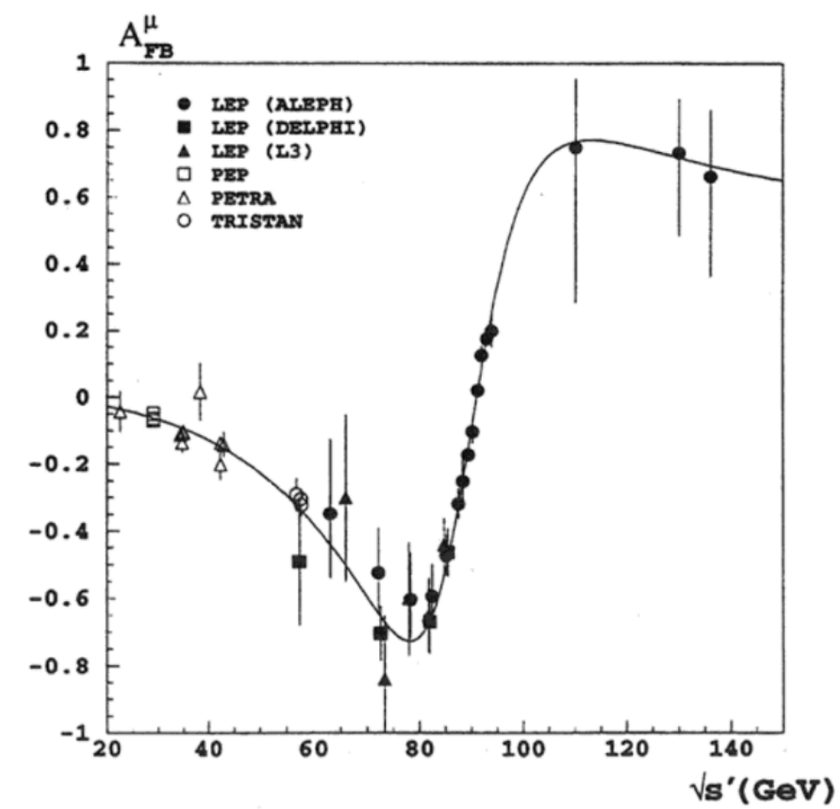


Figure 2: Measured forward-backward asymmetries of muon-pair production compared with the model independent fit results.

CONCLUSIONS

The developments in machine learning and AI go way beyond improved classifiers and have the potential to revolutionize high energy & nuclear physics

- generative models and likelihood-free inference are two particularly exciting areas

Our understanding of how to leverage our prior physics knowledge while letting machine learning do what it's good at is maturing.

- exploit hierarchical structure of events
- individually validated & reusable components

Harnessing the full potential of these techniques will require deep integration into our software and changes to our computing models

Backup / Reference

THE CRUX, AN INTRACTABLE INTEGRAL

Monte Carlo Sampling

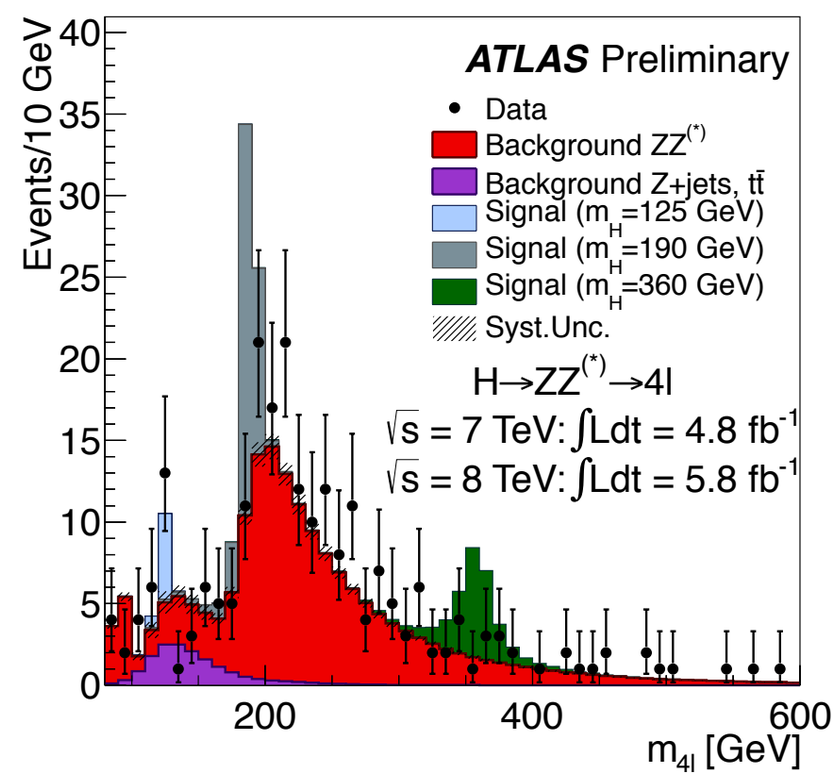
observed

MC Truth

$$p(x|\theta) = \int dz\, p(x, z|\theta)$$

$$\hat{p}(x|\theta)$$

histogram approximation



‘Likelihood-Free’ Inference

← exact Bayesian Computation

Rejection Algorithm

- Draw θ from prior $\pi(\cdot)$
- Accept θ with probability $\pi(D \mid \theta)$

Accepted θ are independent draws from the posterior distribution, $\pi(\theta \mid D)$.

If the likelihood, $\pi(D|\theta)$, is unknown:

‘Mechanical’ Rejection Algorithm

- Draw θ from $\pi(\cdot)$
- Simulate $X \sim f(\theta)$ from the computer model
- Accept θ if $D = X$, i.e., if computer output equals observation

The acceptance rate is $\int \mathbb{P}(D|\theta)\pi(\theta)\mathrm{d}\theta = \mathbb{P}(D)$.

*From Richard Wilkinson’s talk at Data science @LHC

Rejection ABC

If $\mathbb{P}(D)$ is small (or D continuous), we will rarely accept any θ. Instead, there is an approximate version:

Uniform Rejection Algorithm

- Draw θ from $\pi(\theta)$
- Simulate $X \sim f(\theta)$
- Accept θ if $\rho(D, X) \leq \epsilon$

ϵ reflects the tension between computability and accuracy.

- As $\epsilon \to \infty$, we get observations from the prior, $\pi(\theta)$.
- If $\epsilon = 0$, we generate observations from $\pi(\theta \mid D)$.

For reasons that will become clear later, we call this *uniform-ABC*.

*From Richard Wilkinson's talk at Data science @LHC

CARL SOFTWARE

http://diana-hep.org/carl/

diana-hep.org

DiscoveryLinks Higgs RooStats ALEPH Apple News Life Stuff ATLAS Wikipedia, inSpire Theory&Practice nyu espace JCSS HCG

Meet F | Jupyter Note... | Weekend rea... | early-career-... | 2016 Electio... | 12-day Event... | Joint meetin... | carl API doc...

Fork me on GitHub

Index

Sub-modules

- `carl.data`
- `carl.distributions`
- `carl.learning`
- `carl.ratios`

Notebooks

- Composing and fitting distributions
- Diagnostics for approximate likelihood ratios
- Likelihood ratios of mixtures of normals
- Parameterized inference from multidimensional data
- Parameterized inference with nuisance parameters

Display a menu

`carl` module

`carl` is a toolbox for likelihood-free inference in Python.

The likelihood function is the central object that summarizes the information from an experiment needed for inference of model parameters. It is key to many areas of science that report the results of classical hypothesis tests or confidence intervals using the (generalized or profile) likelihood ratio as a test statistic. At the same time, with the advance of computing technology, it has become increasingly common that a simulator (or generative model) is used to describe complex processes that tie parameters of an underlying theory and measurement apparatus to high-dimensional observations. However, directly evaluating the likelihood function in these cases is often impossible or is computationally impractical.

In this context, the goal of this package is to provide tools for the likelihood-free setup, including likelihood (or density) ratio estimation algorithms, along with helpers to carry out inference on top of these.

This project is still in its early stage of development. Join us on GitHub if you feel like contributing!

build passing | coverage 91% | DOI 10.5281/zenodo.47798

Likelihood-free inference with calibrated classifiers

Extensive details regarding likelihood-free inference with calibrated classifiers can be found in the companion paper *"Approximating Likelihood Ratios with Calibrated Discriminative Classifiers", Kyle Cranmer, Juan Pavez, Gilles Louppe.* http://arxiv.org/abs/1506.02169

Installation

The following dependencies are required:

- Numpy >= 1.11

For CARL: see K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

Unifying generative models and exact likelihood-free inference with conditional bijections

By *Kyle Cranmer*, *Gilles Louppe*

machine learning | likelihood-free inference | density estimation

Recent work in density estimation uses a bijection $f : X \to Z$ (e.g. an invertible flow or autoregressive model) and a tractable density $p(z)$ (e.g. [1] [2] [3] [4]).

$$p(x) = p(f_\phi(x)) \left| \det \left(\frac{\partial f_\phi(x)}{\partial x_T} \right) \right| ,$$

where ϕ are the internal network parameters for the bijection f_ϕ. Learning proceeds via gradient ascent $\nabla_\phi \sum_i \log p(x_i)$ with data x_i (i.e. maximum likelihood wrt. the internal parameters ϕ). Since f is invertible, then this model can also be used as a generative model for X.

This can be generalized to the conditional density $p(x|\theta)$ by utilizing a family of bijections $f_\theta : X \to Z$ parametrized by θ (e.g. [5] [6]).

$$p(x|\theta) = p(f_{\phi;\theta}(x)) \left| \det \left(\frac{\partial f_{\phi;\theta}(x)}{\partial x_T} \right) \right|$$

Here θ and x are input to the network (and its inverse) and ϕ are internal network parameters. Again, learning proceeds via gradient ascent $\nabla_\phi \sum_i \log p(x_i|\theta_i)$ with data x_i, θ_i.

We observe that not only can this model be used as a conditional generative model $p(x|\theta)$, but it can also be used to perform asymptotically exact, amortized likelihood-free inference on θ.

This is particularly interesting when θ is identified with the parameters of an intractable, non-differentiable computer simulation or the conditions of some real world data collection process.

Comments

Many thanks to Durk Kingma, Max Welling, Ian Goodfellow, and Shakir Mohamed for enlightening discussions at NIPS2016.

Kyle Cranmer · 9 Dec, 2016

Authors

Kyle Cranmer, Gilles Louppe

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Published: 8 Dec, 2016

BAYES OPT IN A NUTSHELL

[slides from Gilles Louppe]

Bayesian optimisation

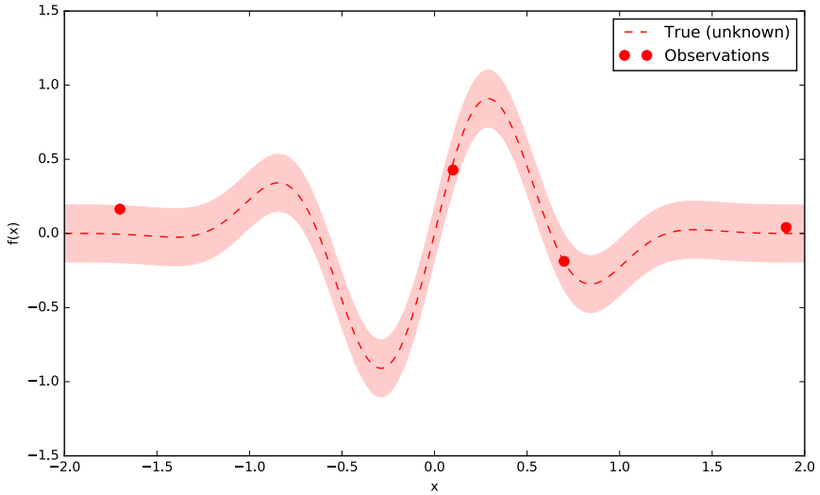
for $t = 1 : T$,

1. Given observations (x_i, y_i) for $i = 1 : t$, build a probabilistic model for the objective f.
   - Integrate out all possible true functions, using Gaussian process regression.
2. Optimise a cheap utility function u based on the posterior distribution for sampling the next point.

$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Where shall we sample next?



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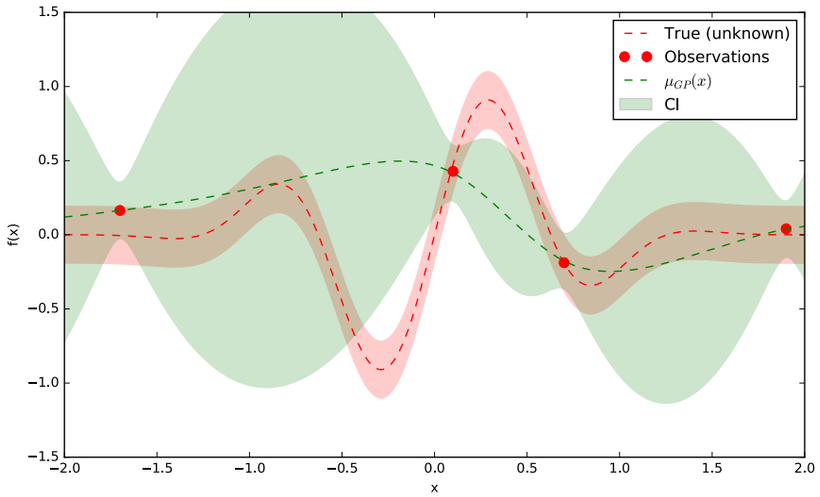
Build a probabilistic model for the objective function



This gives a posterior distribution over functions that could have generated the observed data.

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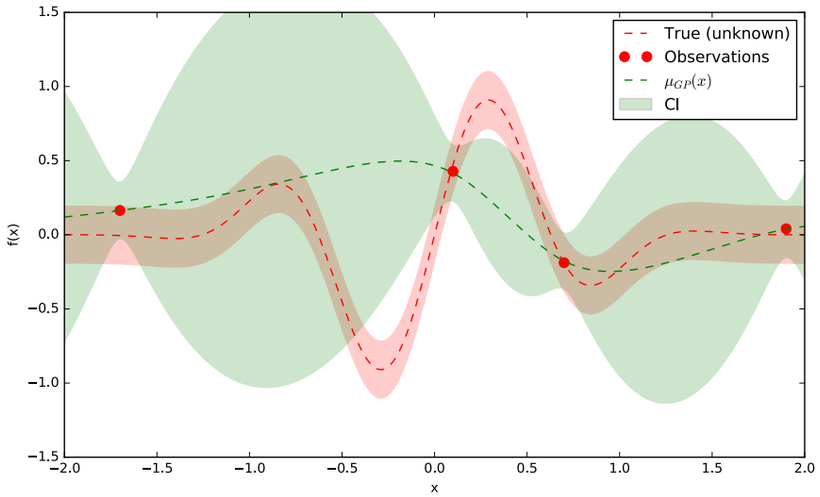


This gives a posterior distribution over functions that could have generated the observed data.

Acquisition functions

Acquisition functions u(x) specify which sample x should be tried next:

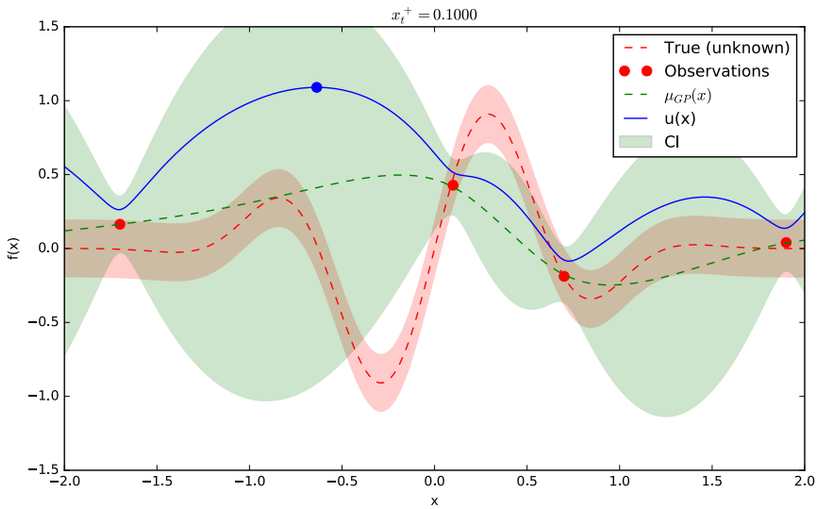
- Upper confidence bound $\text{UCB}(x) = \mu_{GP}(x) + \kappa\sigma_{GP}(x)$;
- Probability of improvement $\text{PI}(x) = P(f(x) \geq f(x_t^+) + \kappa)$;
- Expected improvement $\text{EI}(x) = \mathbb{E}[f(x) - f(x_t^+)]$;
- ... and many others.

where x_t^+ is the best point observed so far.

In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

Plugging everything together ($t = 0$)



$$x_{t+1} = \arg\max_x \text{UCB}(x)$$

BAYES OPT IN A NUTSHELL

[slides from Gilles Louppe]

Bayesian optimisation

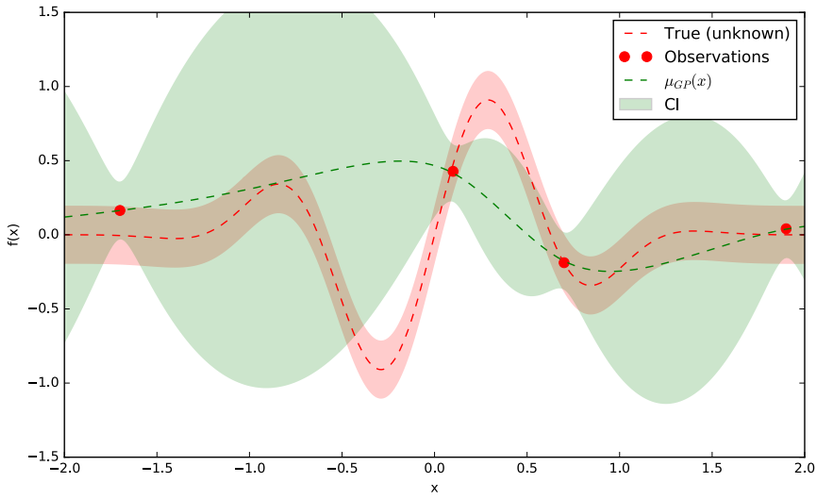
for $t = 1 : T$,

1. Given observations (x_i, y_i) for $i = 1 : t$, build a probabilistic model for the objective f.
   - Integrate out all possible true functions, using Gaussian process regression.
2. Optimise a cheap utility function u based on the posterior distribution for sampling the next point.

$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Build a probabilistic model for the objective function



This gives a posterior distribution over functions that could have generated the observed data.

Acquisition functions

Acquisition functions u(x) specify which sample x should be tried next:

- Upper confidence bound $\text{UCB}(x) = \mu_{GP}(x) + \kappa\sigma_{GP}(x)$;
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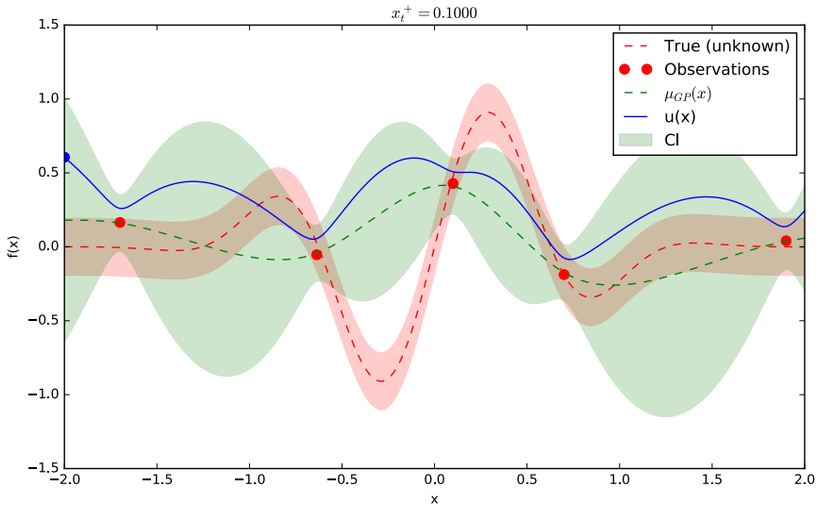
- Expected improvement $\text{EI}(x) = \mathbb{E}[f(x) - f(x_t^+)]$;
- ... and many others.

where x_t^+ is the best point observed so far.

In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

... and repeat until convergence ($t = 1$)



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[slides from Gilles Louppe]

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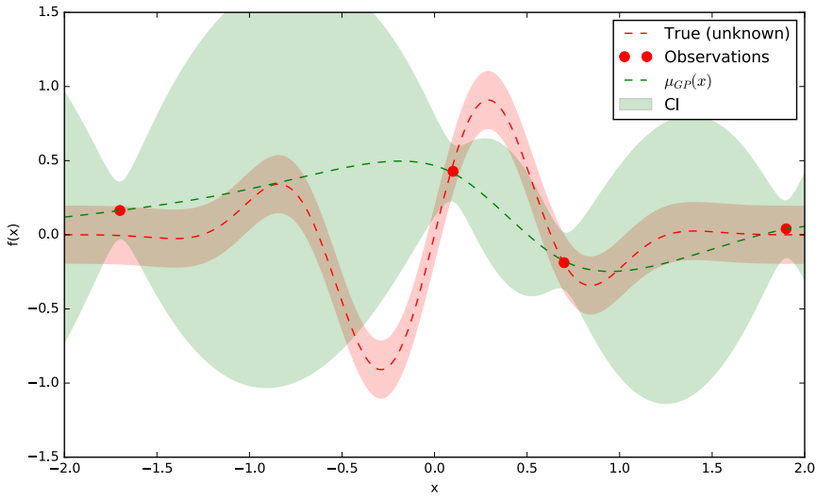
$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Build a probabilistic model for the objective function



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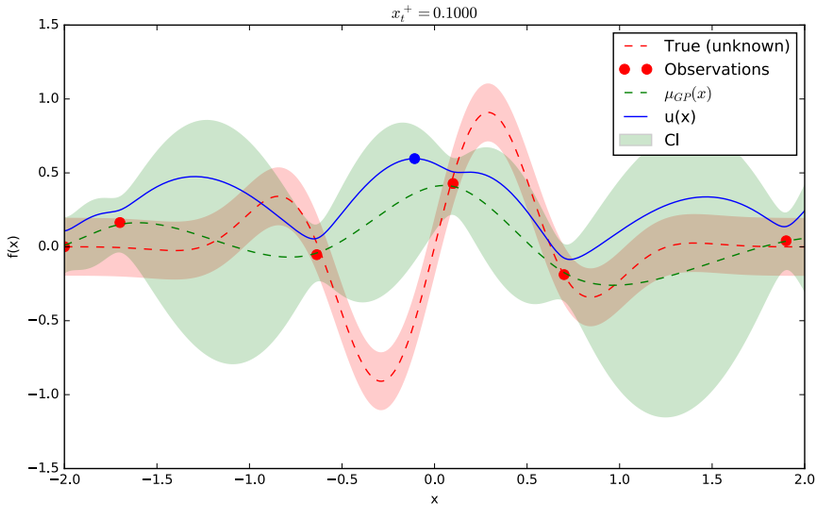
- ... and many others.

where x_t^+ is the best point observed so far.

In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

... and repeat until convergence ($t = 2$)



BAYES OPT IN A NUTSHELL

[slides from Gilles Louppe]

Bayesian optimisation

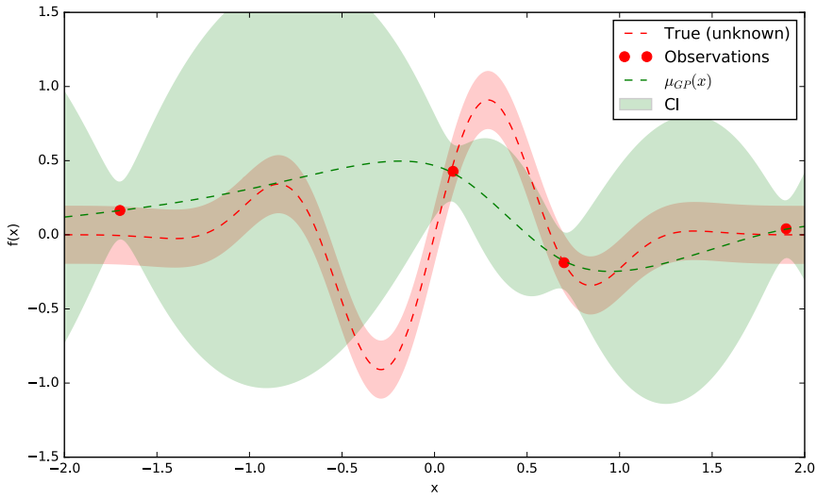
for $t = 1 : T$,

1. Given observations (x_i, y_i) for $i = 1 : t$, build a probabilistic model for the objective f.
   - Integrate out all possible true functions, using Gaussian process regression.
2. Optimise a cheap utility function u based on the posterior distribution for sampling the next point.

$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Build a probabilistic model for the objective function



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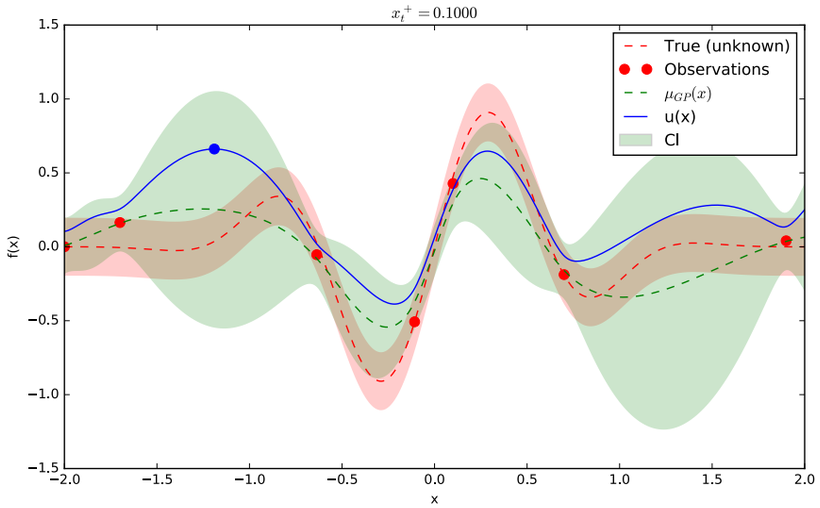
- ... and many others.

where x_t^+ is the best point observed so far.

In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

... and repeat until convergence ($t = 3$)



BAYES OPT IN A NUTSHELL

[slides from Gilles Louppe]

Bayesian optimisation

for $t = 1 : T$,

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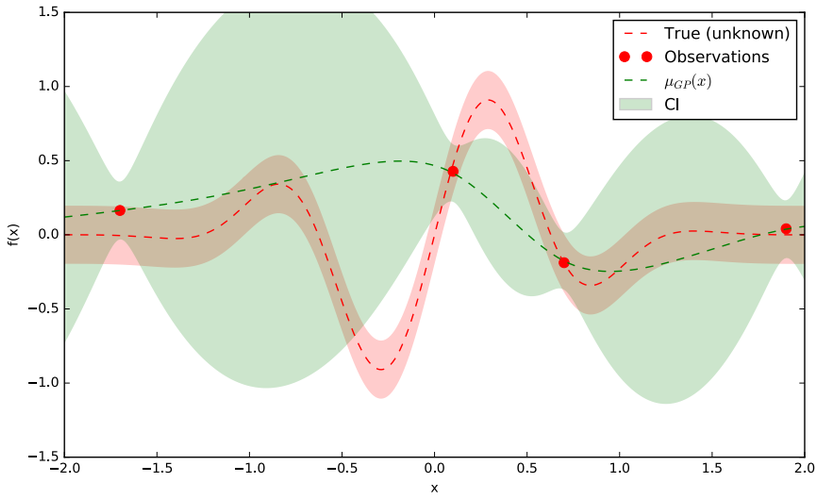
$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Build a probabilistic model for the objective function



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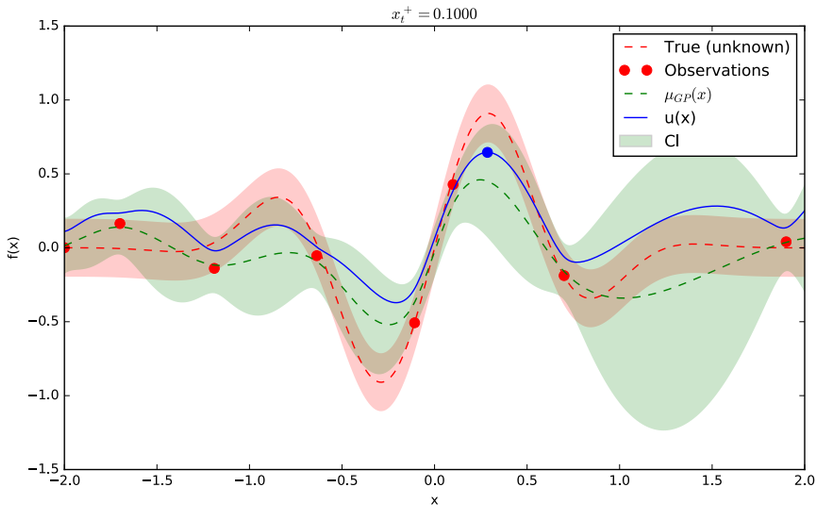
where x_t^+ is the best point observed so far.

In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

... and repeat until convergence ($t = 4$)



BAYES OPT IN A NUTSHELL

[slides from Gilles Louppe]

Bayesian optimisation

for $t = 1 : T$,

1. Given observations (x_i, y_i) for $i = 1 : t$, build a probabilistic model for the objective f.
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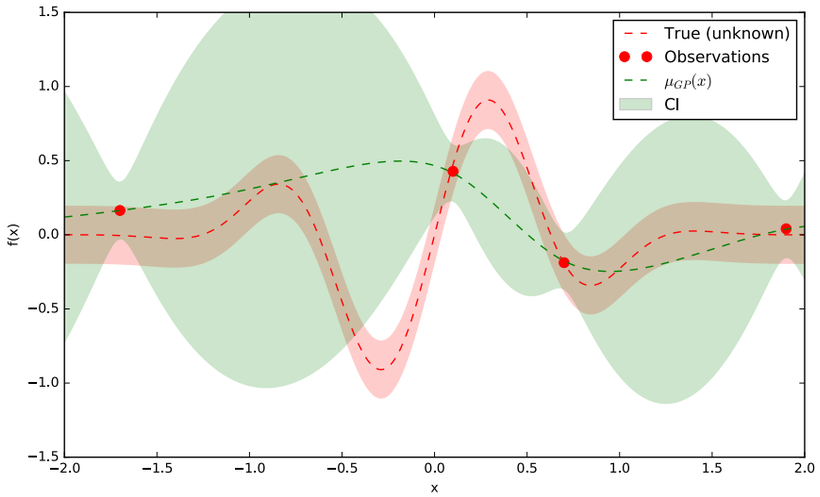
2. Optimise a cheap utility function u based on the posterior distribution for sampling the next point.

$$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}.

Build a probabilistic model for the objective function



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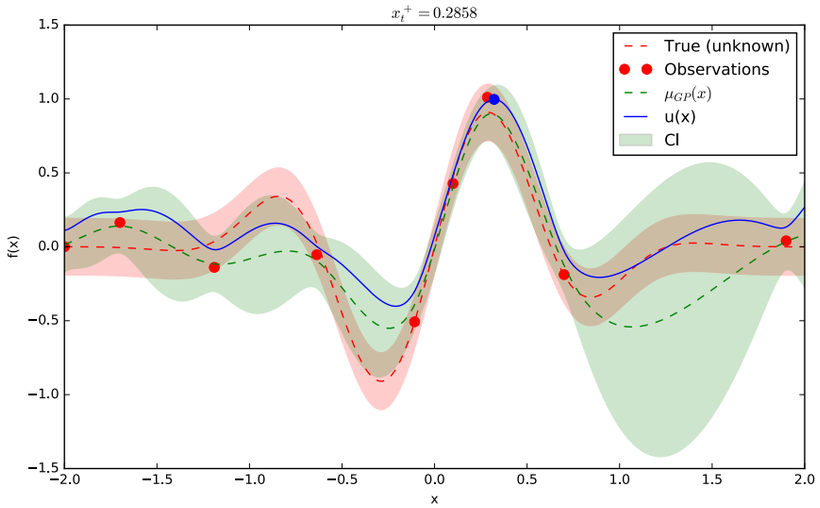
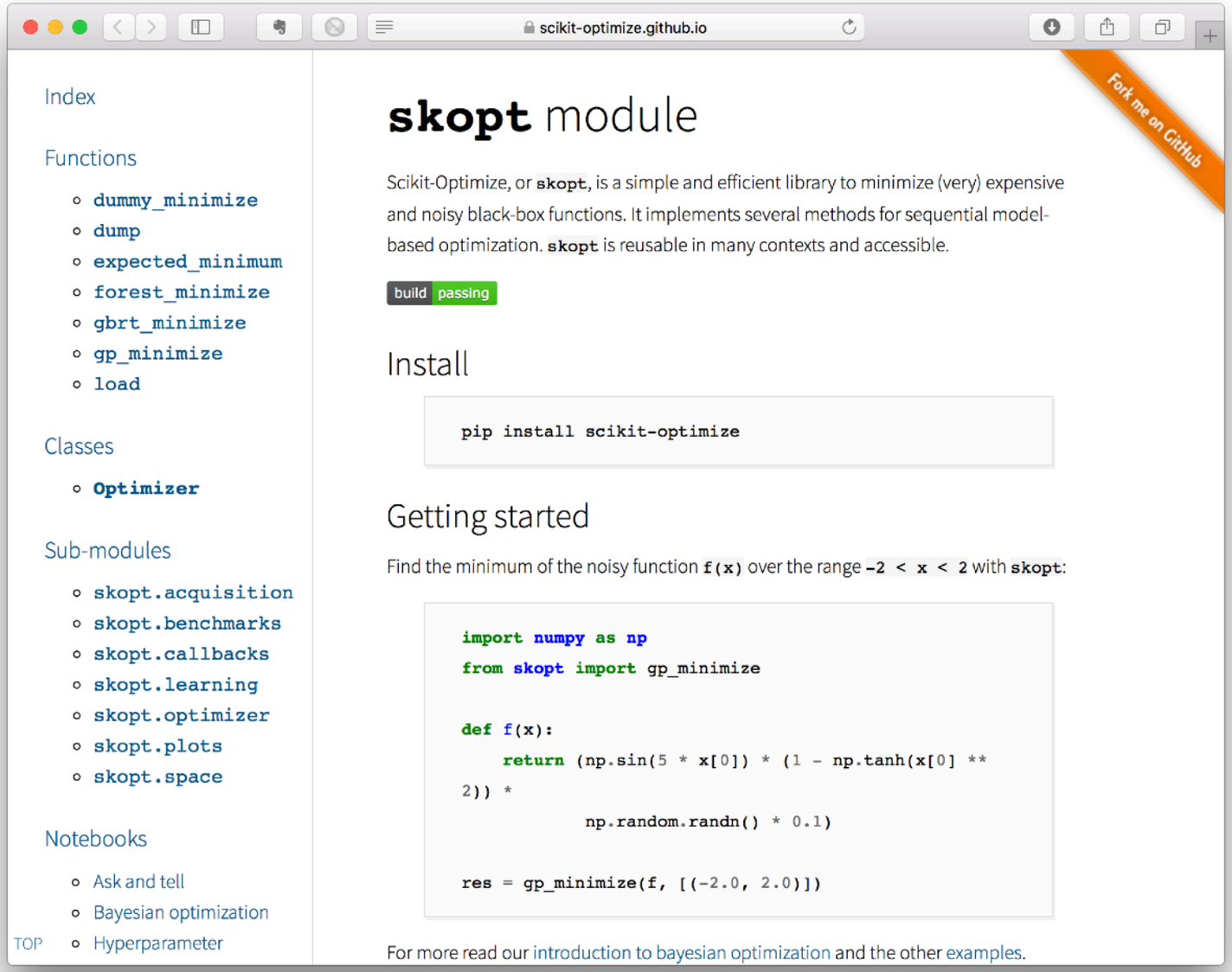
- Search in regions where $\mu_{GP}(x)$ is high (exploitation)
- Probe regions where uncertainty $\sigma_{GP}(x)$ is high (exploration)

... and repeat until convergence ($t = 5$)



OPTIMIZATION SOFTWARE

- Python
  - Spearmint https://github.com/JasperSnoek/spearmint
  - GPyOpt https://github.com/SheffieldML/GPyOpt
  - RoBO https://github.com/automl/RoBO
  - scikit-optimize https://github.com/MechCoder/scikit-optimize (work in progress)
- C++
  - MOE https://github.com/yelp/MOE



GitHub Repo for previous slides:
https://github.com/glouppe/talk-bayesian-optimisation

SOFTWARE

Yadage and Packtivity – analysis preservation using parametrized workflows

Kyle Cranmer[1] **and Lukas Heinrich**[1]

[1] Department of Physics, New York University, New York, USA

E-mail: `lukas.heinrich@cern.ch`

Abstract. Preserving data analyses produced by the collaborations at LHC in a parametrized fashion is crucial in order to maintain reproducibility and re-usability. We argue for a declarative description in terms of individual processing steps – "packtivities" – linked through a dynamic directed acyclic graph (DAG) and present an initial set of JSON schemas for such a description and an implementation – "yadage" – capable of executing workflows of analysis preserved via Linux containers.

GitHub, Inc.

yadage - yaml based adage

DOI 10.5281/zenodo.309288 | pypi package 0.10.8 | build passing | health 94% | coverage 90% | docs latest | version git-master

A declarative way to define adage workflows using a JSON schema (but we'll always write it as YAML)

```
docker run --rm -it -v /var/run/docker.sock:/var/run/docker.sock -v $PWD:$PWD -w $PWD lukasheinrich/yada
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

or just

```
eval "$(curl https://raw.githubusercontent.com/diana-hep/yadage/master/yadagedocker.sh)"
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

This package reads and executes workflows adhering to the workflow JSON schemas defined at https://github.com/diana-hep/cap-schemas such as the onces stored in the community repository https://github.com/lukasheinrich/yadage-workflows. For executing the individual steps it mainly uses the packtivity python bindings provided by https://github.com/diana-hep/packtivity.

Possible Backends:

Yadage can run on various backends such as multiprocessing pools, ipython clusters, or celery clusters. If human intervention is needed for certain steps, it can also be run interactively.

Example Workflow

```
stages:
  - name: hello_world
```

reana.readthedocs.io

Fork me on GitHub

REANA - Reusable Analyses

build passing | coverage 100% | docs latest | Issues ready for work 2 | gitter join chat | license GNU General Public License v2.0

REANA is a system that permits to instantiate research data analyses on the cloud. It uses container-based technologies and was born to target the use case of particle physics analyses in LHC collaborations. The system paves the way to reusing and reinterpreting preserved data analyses even several years after the original analysis.

REANA - Reusable Analyses

Navigation

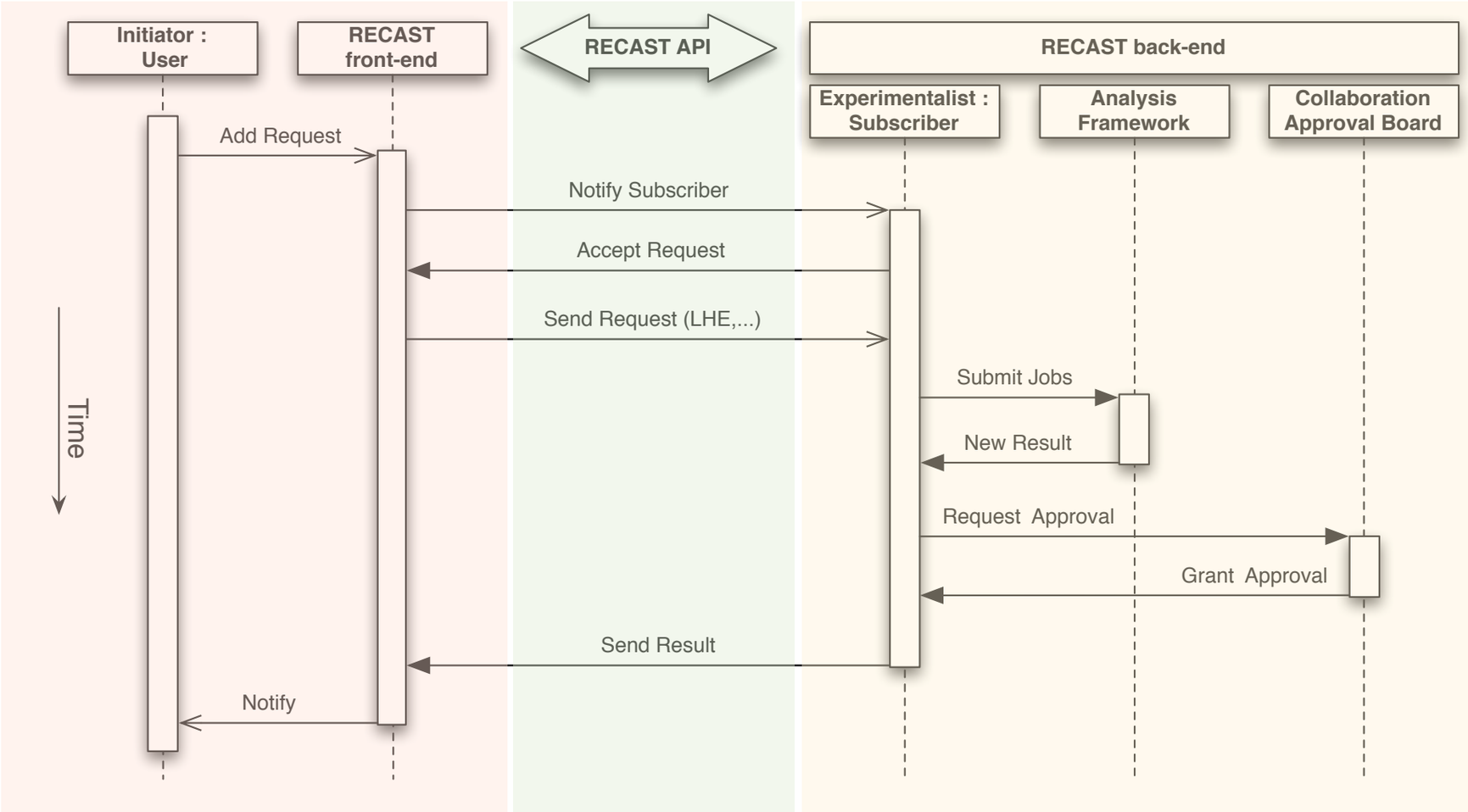
REANA@DockerHub
REANA@GitHub

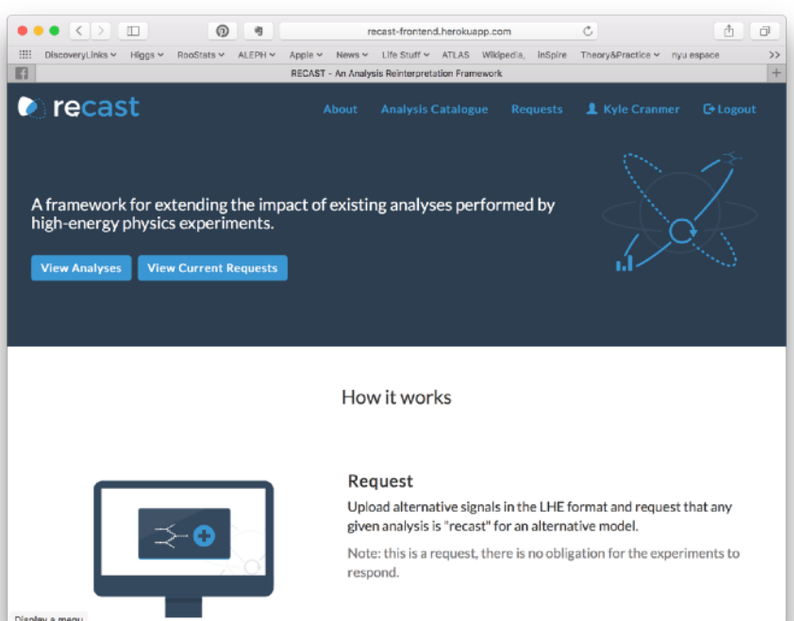
Quick search

Go

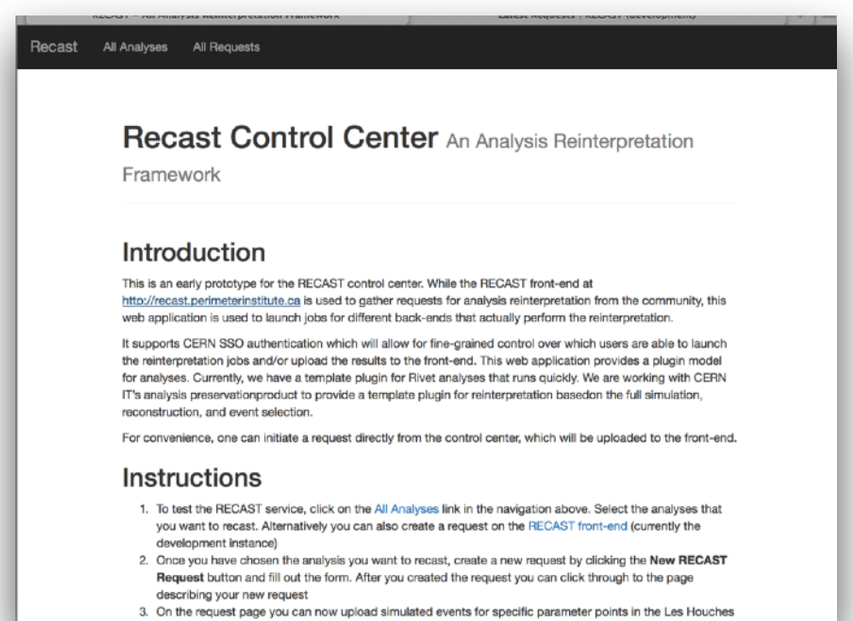
v: latest

https://arxiv.org/pdf/1706.01878.pdf

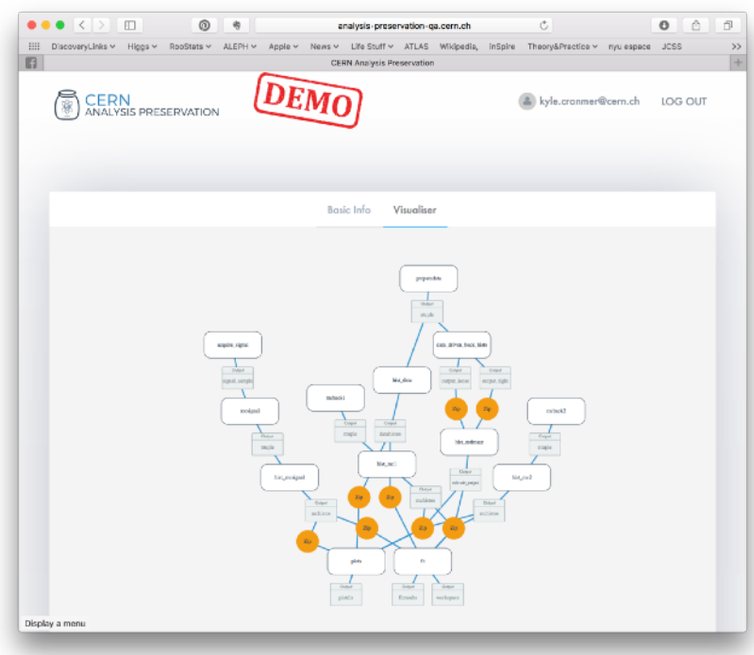




Front-End: public facing
collects requests



Control Center: not public, uses CERN auth.,
oversees processing of jobs on back-end



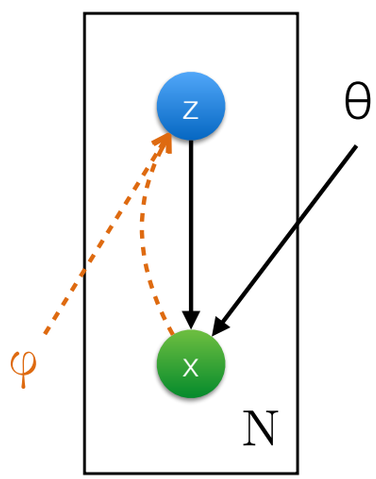
CERN Analysis Preservation:
Stores workflows, provides back-end
computing resources

VARIATIONAL AUTO-ENCODER

[Slides from D. Kingma NIPS 2015]

Auto-Encoding Variational Bayes

[Kingma and Welling, 2013/2014]
[Rezende et al, 2014]



- $q_\varphi(z|x) = N(\mu,\sigma^2)$
  $[\mu, \sigma^2] = f^{(z|x)}(x,\varphi) = \text{multilayer neural net}$
- Objective: lower bound of log p(x).
  - Jointly optimized w.r.t. φ and θ
  - This is approx. maximum likelihood
  - Simple SGD:
    - Sampling small minibatches of data
    - Sampling from approx. posterior
- This also minimizes an expected KL divergence
  $D_{KL}(q_\varphi(z|x)||p(z|x))$
  -> gives us cheap approx. inference for new datapoints

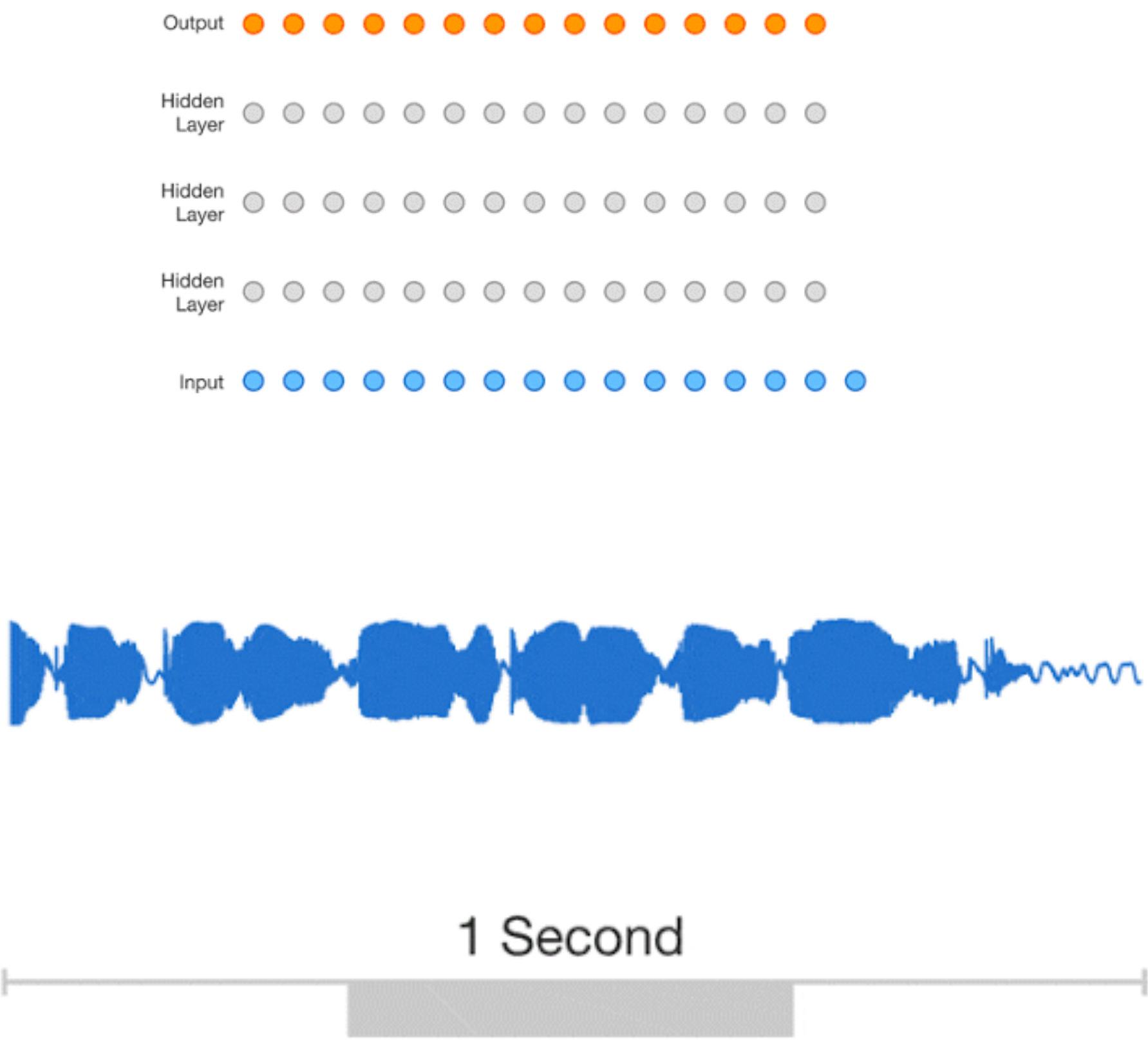
Diederik (Durk) Kingma

Max Welling

Conv. net as encoder/decoder, trained on faces

Kingma and Welling, Auto-encoding Variational Bayes, ICLR 2014
Rezende, Mohamed and Wierstra, Stochastic back-propagation and variational inference in deep latent Gaussian models, ICML 2014

WAVENET: A GENERATIVE MODEL FOR RAW AUDIO



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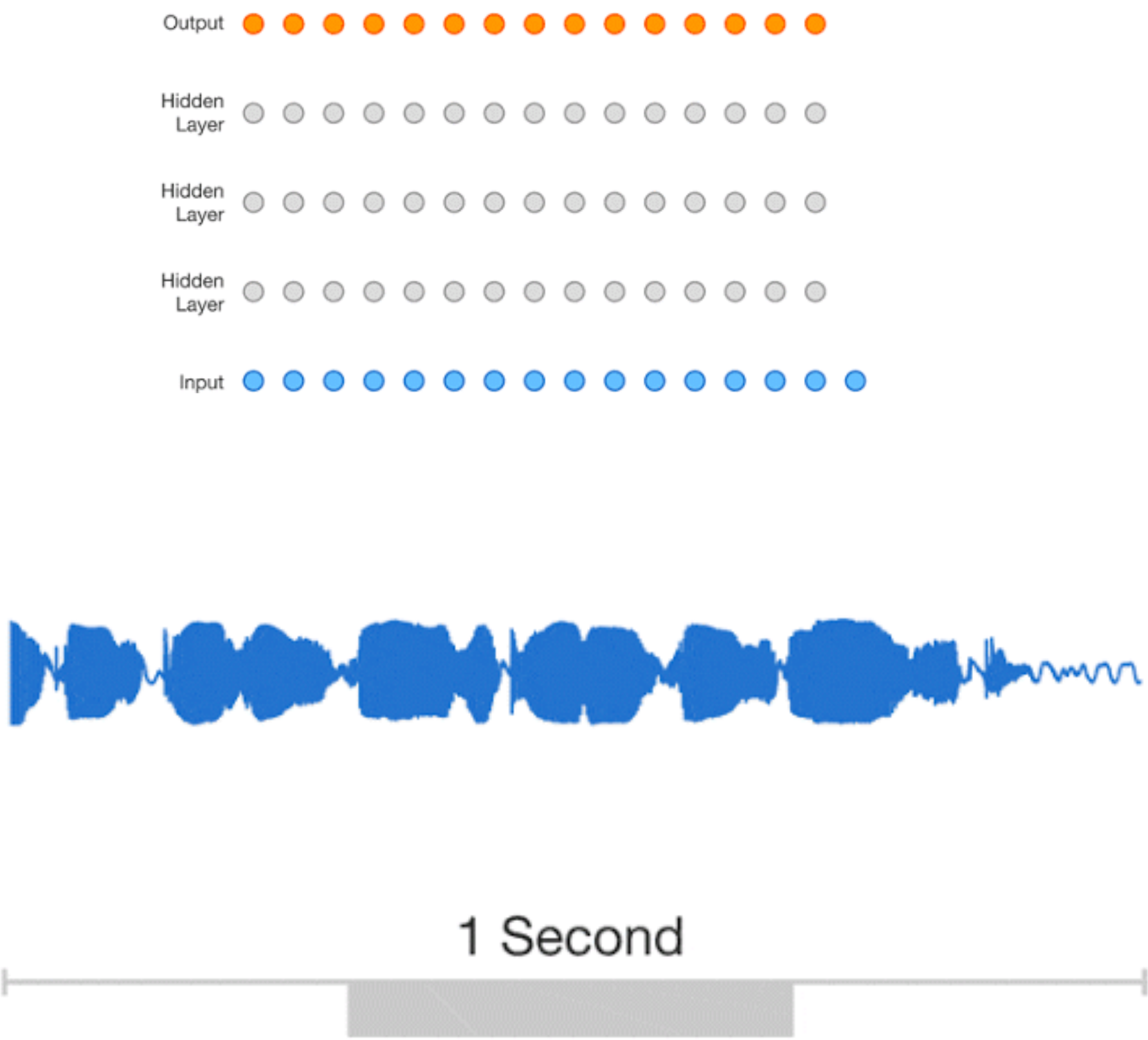

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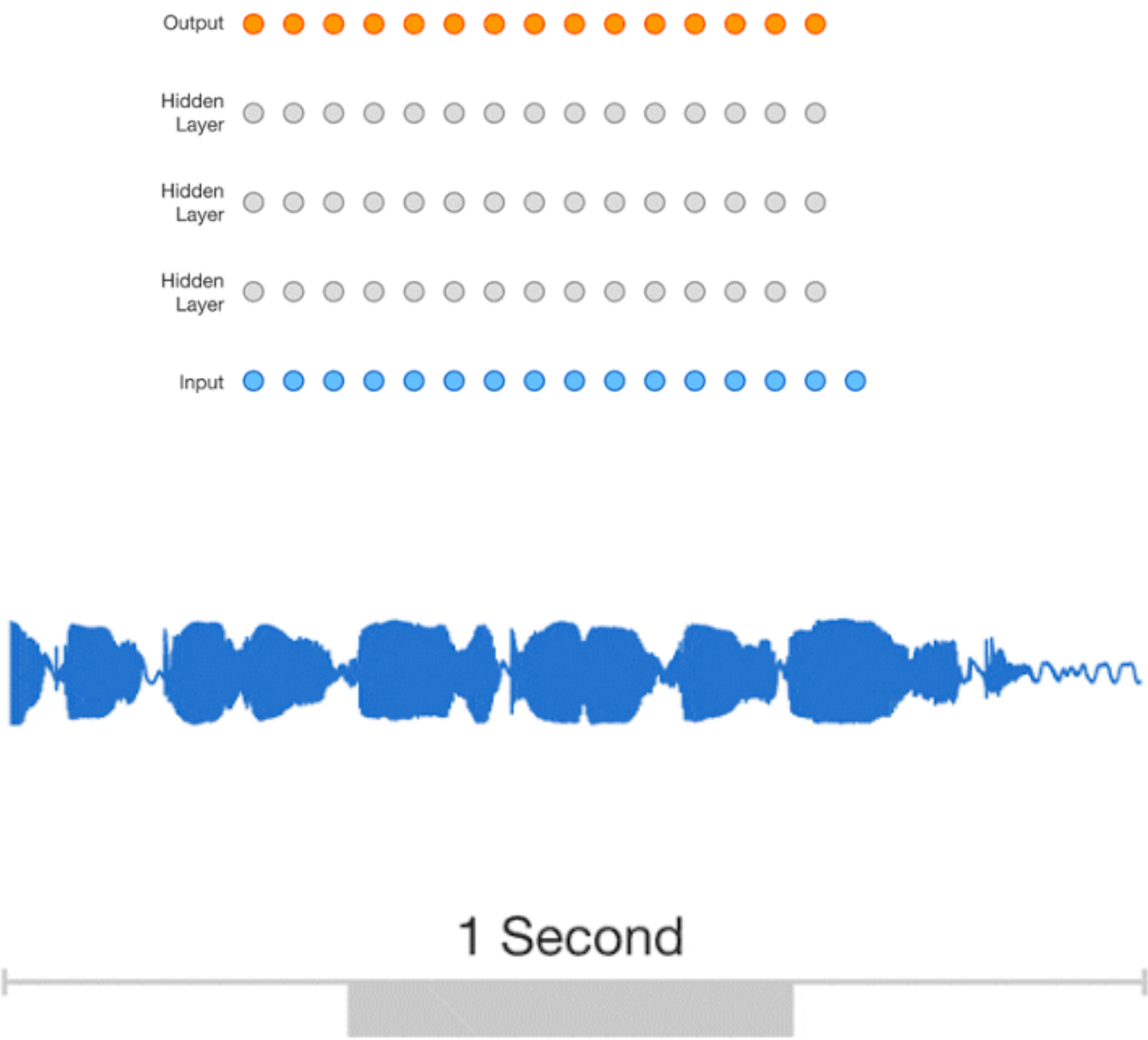


Create standalone simulation tools to facilitate collaboration between HEP and machine learning community

By Pierre Baldi, Peter Sadowski, Daniel Whiteson, Christian Lorenz Müller, Michael Williams, Lukas Heinrich, Steven Schramm, Maurizio Pierini, Sergei Gleyzer, Amir Farbin, jean-roch vlimant, Tim Head, Juan Pavez, Peter Elmer, Balázs Kégl, Andrey Ustyuzhanin, Vladimir Gligorov, Gilles Louppe, Kyle Cranmer

dslhc | machinelearning | datascience | open data | simulation

Discussions at recent workshops have made it clear that one of the key barriers to collaboration between high energy physics and the machine learning community is access to training data. Recent successes in data sharing through the HiggsML and Flavours of Physics Kaggle challenges have borne much fruit, but required significant effort to coordinate.

While static simulated datasets are useful for challenges, in the course of investigating new machine learning techniques it is advantageous to be able to generate training data on demand (e.g. Refs. 1, 2, 3).
Therefore we recommend efforts be made to produce the ingredients required to facilitate such collaboration:

- Specific challenges for HEP experiments should be fully specified such that minimal domain-specific knowledge is required to attack them.
- Stand-alone simulators should be made open source. They should be developed to be easy to use without domain-specific expertise, while still being representative of real experimental challenges. Such a simulation will permit non-HEP researchers to generate realistic HEP datasets for training and testing. These simulators could range from truth-level simulation of a hard scattering to fast simulation like Delphes, to full GEANT4 simulation of sensor arrays.
- Performance metrics (objective functions) and operational constraints should be defined to evaluate proposed solutions.

Authors

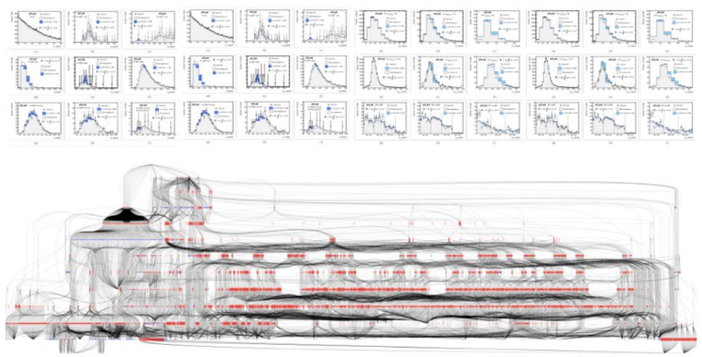
Pierre Baldi, Peter Sadowski, Daniel Whiteson, Christian Lorenz Müller, Michael Williams, Lukas Heinrich, Steven Schramm, Maurizio Pierini, Sergei Gleyzer, Amir Farbin, jean-roch vlimant, Tim Head, Juan Pavez, Peter Elmer, Balázs Kégl, Andrey Ustyuzhanin, Vladimir Gligorov, Gilles Louppe, Kyle Cranmer

Metadata

DOI 10.5281/zenodo.46864

Published: 26 Feb, 2016

Probabilistic programming frameworks

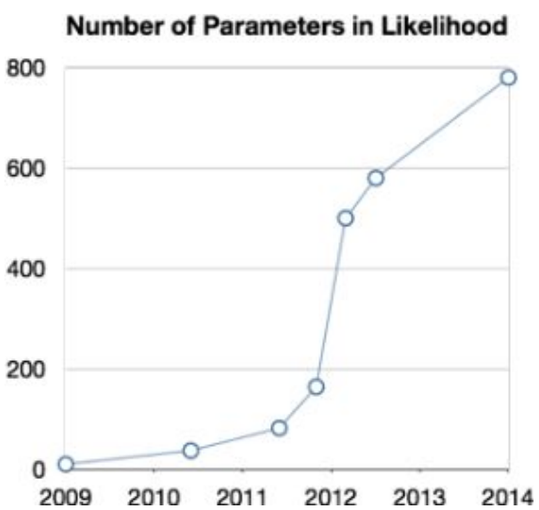


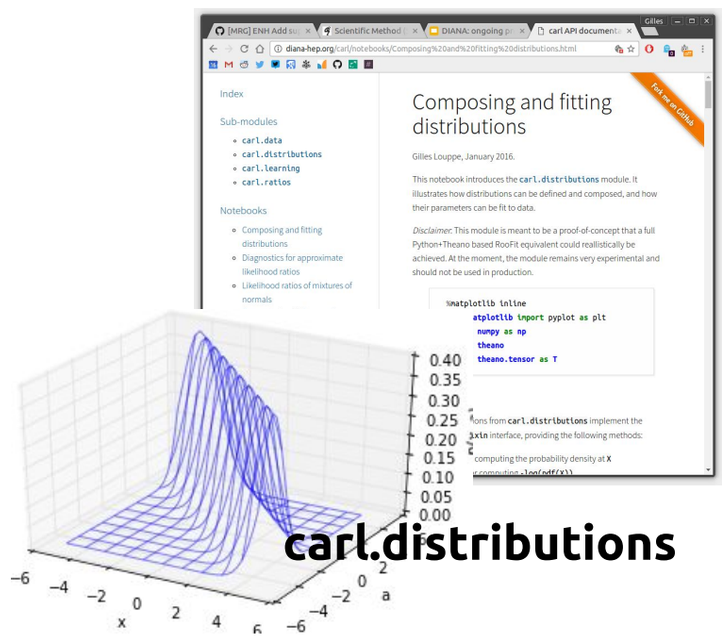
$$\mathbf{f}_{\text{tot}}(\mathcal{D}_{\text{sim}}, \mathcal{G}|\boldsymbol{\alpha}) = \prod_{c \in \text{channels}} \left[\text{Pois}(n_c|\nu_c(\boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_{ce}|\boldsymbol{\alpha}) \right] \cdot \prod_{p \in \mathbb{S}} f_p(a_p|\alpha_p)$$

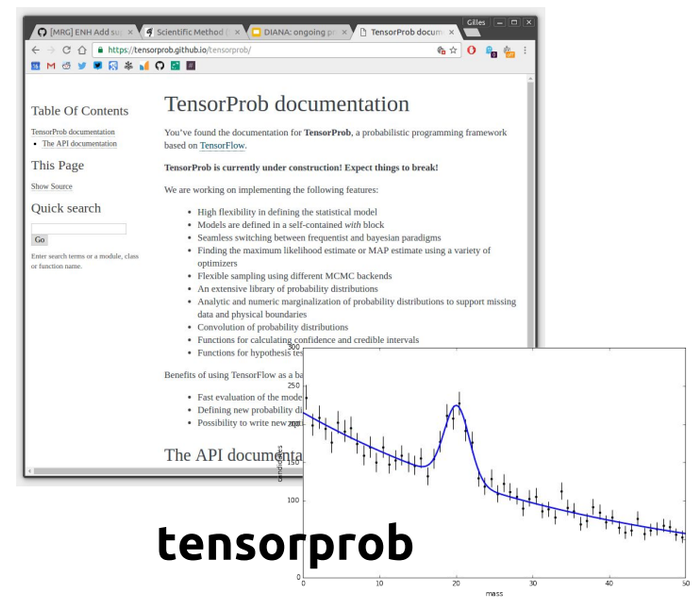
RooFit serves us well, but shows limits in terms of **scalability**.

Using a data flow graph framework, RooFit would be **distributed**, **GPU-enabled** and automatically **differentiable**.

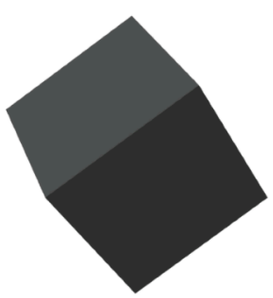
Feasibility? Certainly **within reach!** As illustrated by our tentative proof-of-concepts carl.distributions [Gilles Louppe] and tensorprob [Igor Babuschkin, now at DeepMind]. See also Edward.







Edward



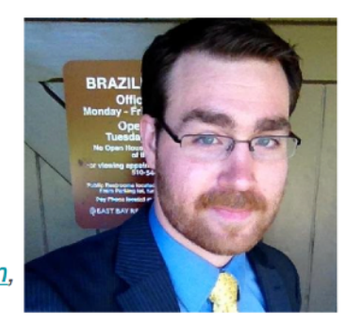
A library for probabilistic modeling, inference, and criticism.

Edward is a Python library for probabilistic modeling, inference, and criticism. It is a testbed for fast experimentation and research with probabilistic models, ranging from classical hierarchical models on small data sets to complex deep probabilistic models on large data sets. Edward fuses three fields: Bayesian statistics and machine learning, deep learning, and probabilistic programming.

It supports **modeling** with

Dustin Tran

Ph.D. Student
Columbia University
dustin@cs.columbia.edu (@dustinvtran, http://dustintran.com



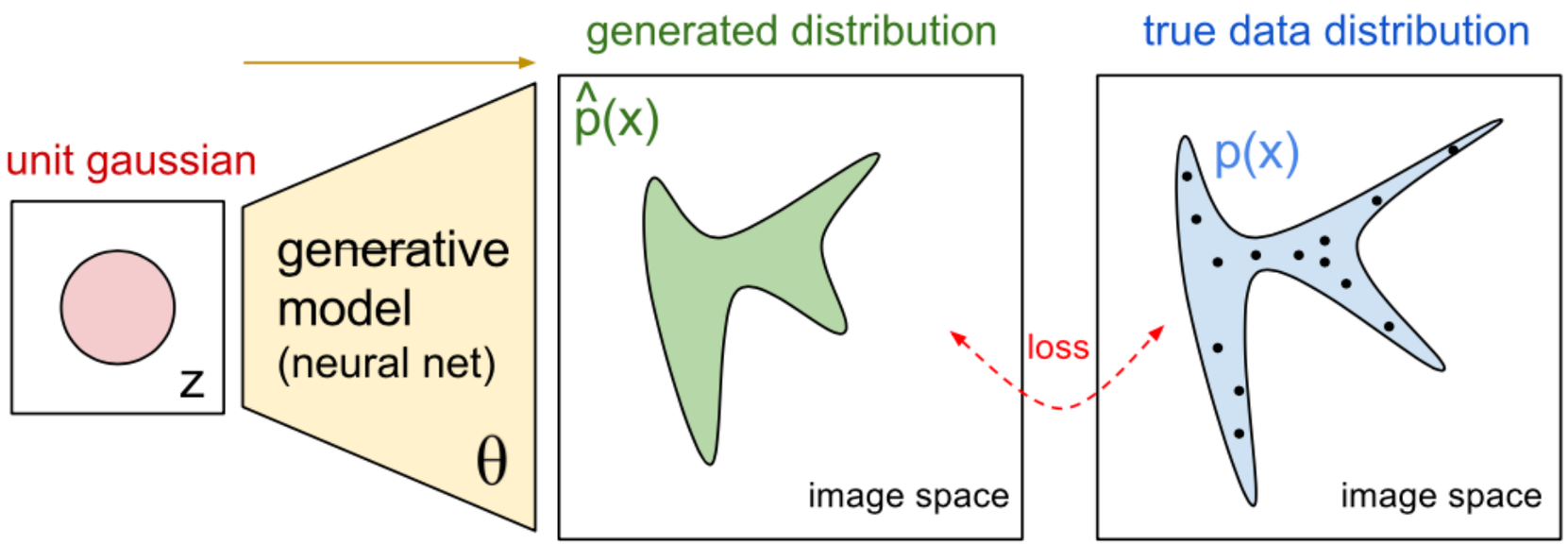
Matthew Feickert

High Energy Physics Ph.D. Candidate
Southern Methodist University
matthew.feickert@cern.ch or mfeickert@smu.edu
GitHub: matthewfeickert @HEPfeickert

Adversarial Training
(not just for GANs)

GENERATIVE ADVERSARIAL NETWORKS

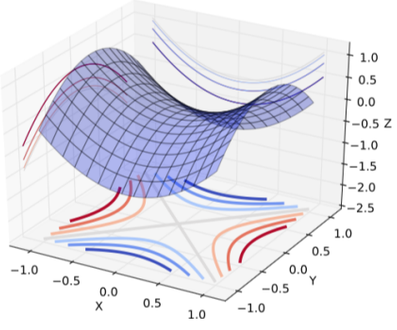
Goodfellow, et al arXiv:1406.2661
slide Gilles Louppe



Leo is G Tom is D

- Two-player game:
  - a discriminator D,
  - a generator G;
- D is a classifier $\mathcal{X} \mapsto \{0, 1\}$ that tries to distinguish between
  - a sample from the data distribution ($D(\mathbf{x}) = 1$, for $\mathbf{x} \sim p_{\text{data}}$),
  - and a sample from the model distribution ($D(G(\mathbf{z})) = 0$, for $\mathbf{z} \sim p_{\text{noise}}$);
- G is a generator $\mathcal{Z} \mapsto \mathcal{X}$ trained to produce samples $G(\mathbf{z})$ (for $\mathbf{z} \sim p_{\text{noise}}$) that are difficult for D to distinguish from data.

$$(D^*, G^*) = \max_D \min_G V(D, G).$$



NEW! AVO

G. Louppe & K.C. arXiv:1707.07113

Adversarial Variational Optimization of Non-Differentiable Simulators

Gilles Louppe[1] and **Kyle Cranmer**[1]
[1]*New York University*

Complex computer simulators are increasingly used across fields of science as generative models tying parameters of an underlying theory to experimental observations. Inference in this setup is often difficult, as simulators rarely admit a tractable density or likelihood function. We introduce Adversarial Variational Optimization (AVO), a likelihood-free inference algorithm for fitting a non-differentiable generative model incorporating ideas from empirical Bayes and variational inference. We adapt the training procedure of generative adversarial networks by replacing the differentiable generative network with a domain-specific simulator. We solve the resulting non-differentiable minimax problem by minimizing variational upper bounds of the two adversarial objectives. Effectively, the procedure results in learning a proposal distribution over simulator parameters, such that the corresponding marginal distribution of the generated data matches the observations. We present results of the method with simulators producing both discrete and continuous data.

Leo is G Tom is D

Similar to GAN setup, but instead of using a neural network as the generator, use the actual simulation (eg. Pythia, GEANT)

Continue to use a neural network discriminator / critic.

Difficulty: the simulator isn't differentiable, but there's a **trick**!

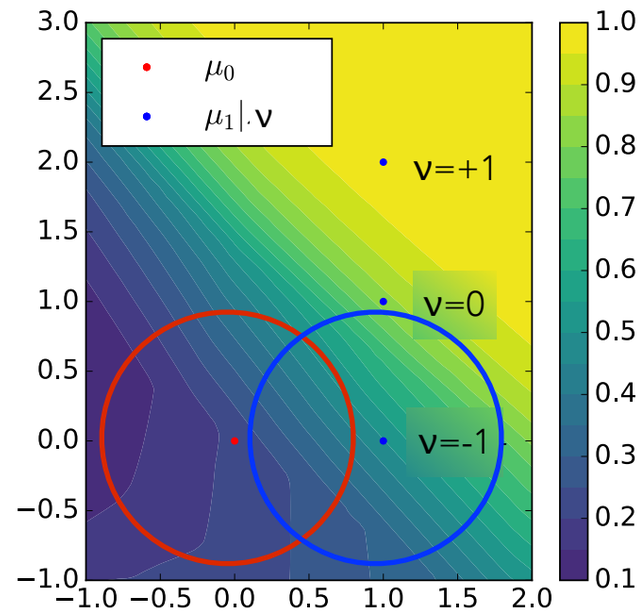
Allows us to efficiently fit / **tune simulation** with stochastic gradient techniques!

LEARNING TO PIVOT WITH ADVERSARIAL NETWORKS

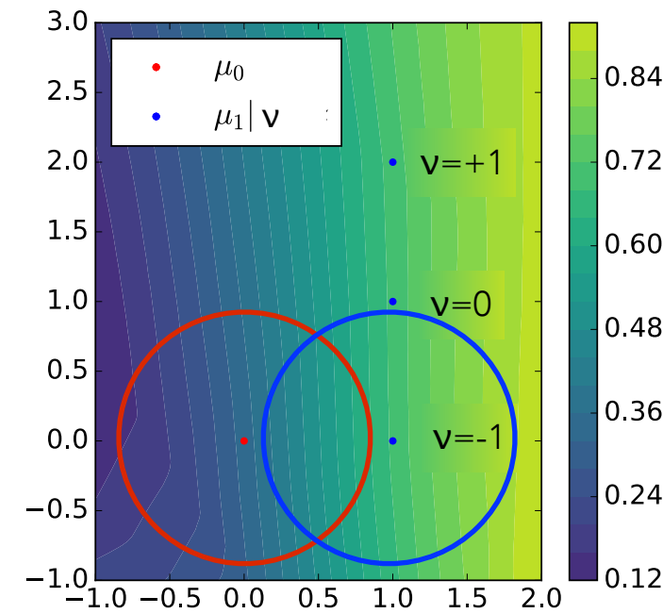
Typically classifier **f(x)** trained to minimize loss $\mathbf{L_f}$.

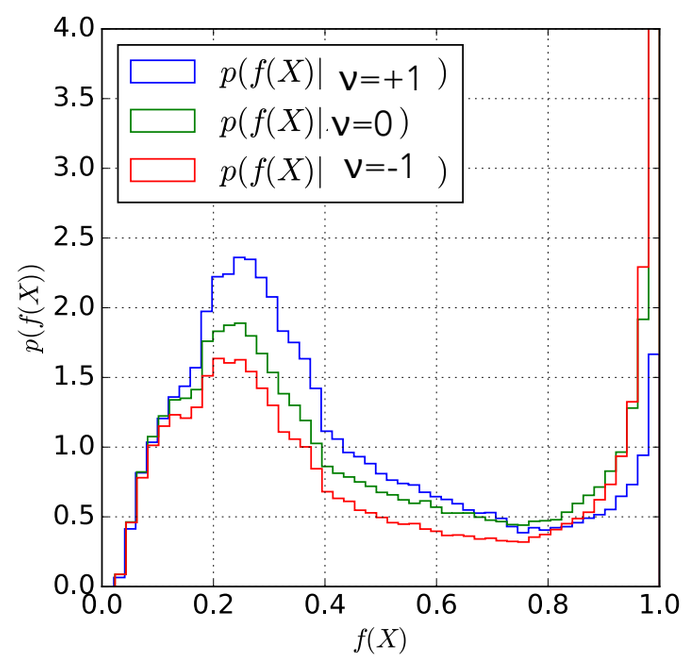
- want classifier output to be insensitive to systematics (nuisance parameter **ν**)
- introduce an **adversary r** that tries to predict ν based on f.
- provides training procedure that allows for **tradeoff** between traditional classification accuracy and **robustness to systematics**

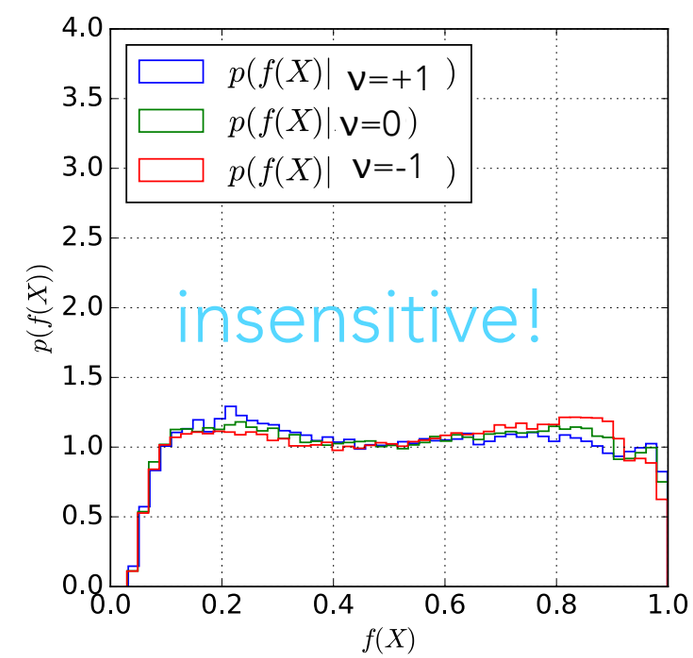
normal training



adversarial training







G. Louppe, M. Kagan, K. Cranmer, arXiv:1611.01046

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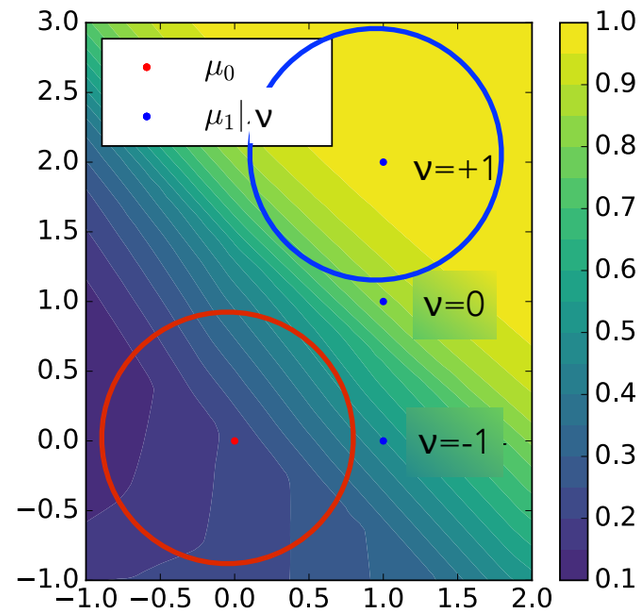
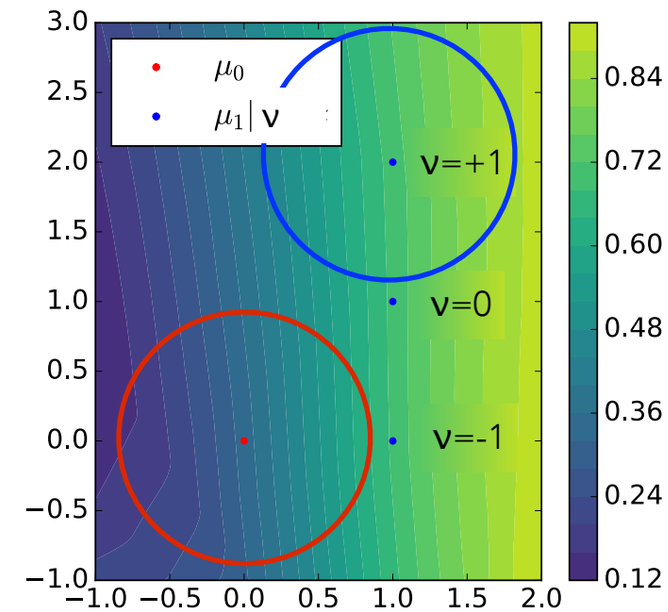
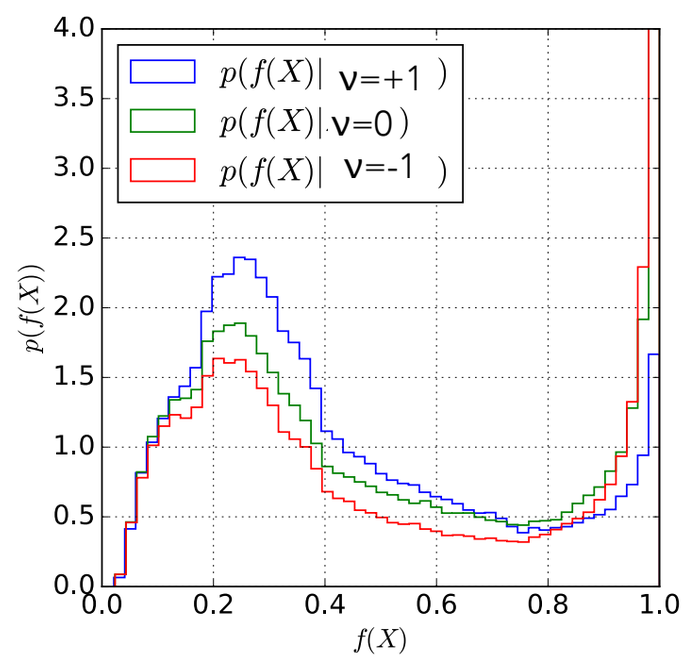
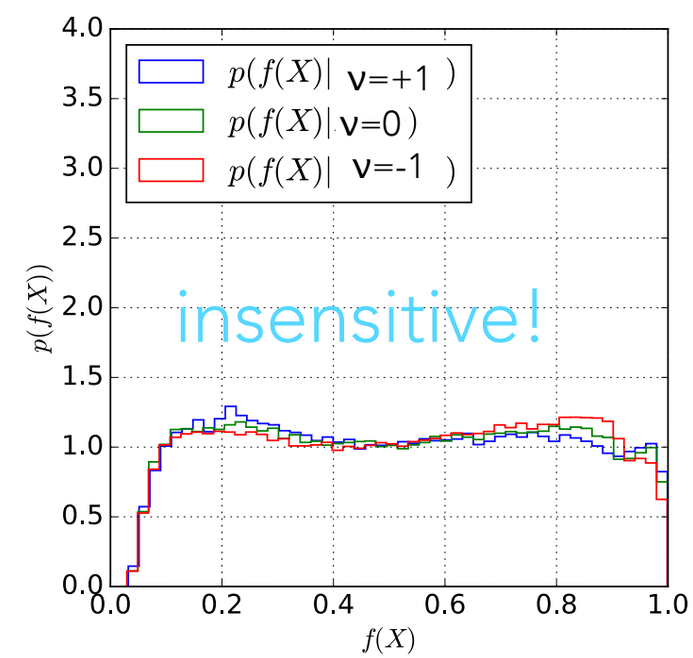


adversarial training







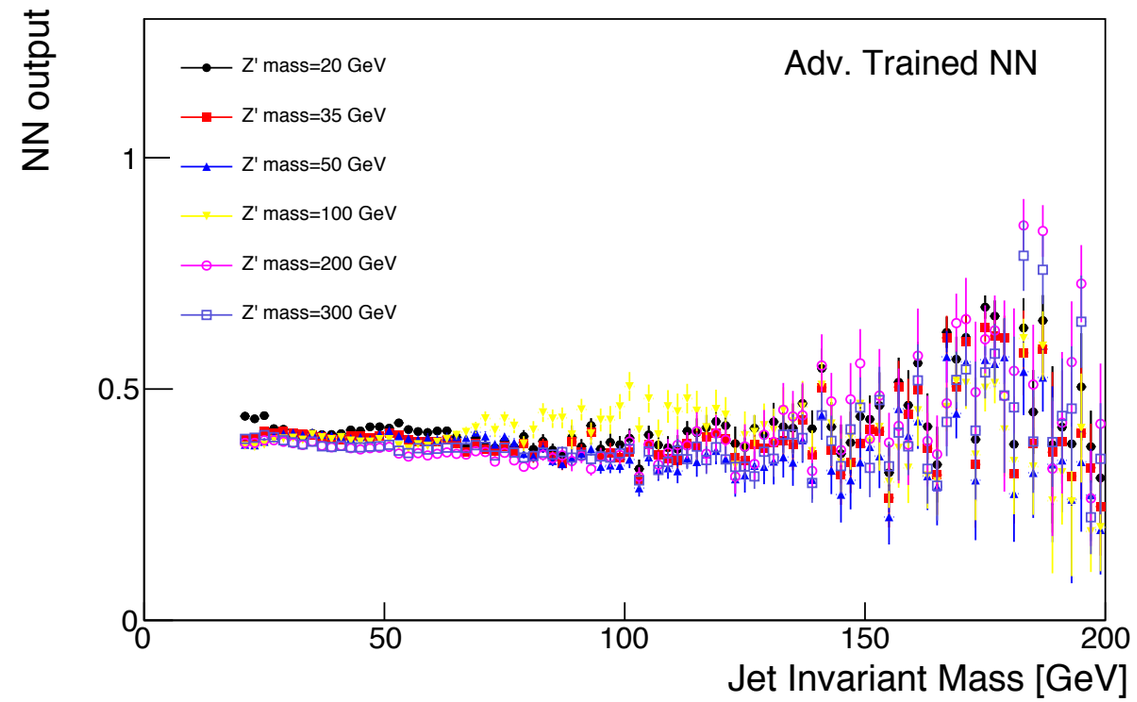
G. Louppe, M. Kagan, K. Cranmer, arXiv:1611.01046

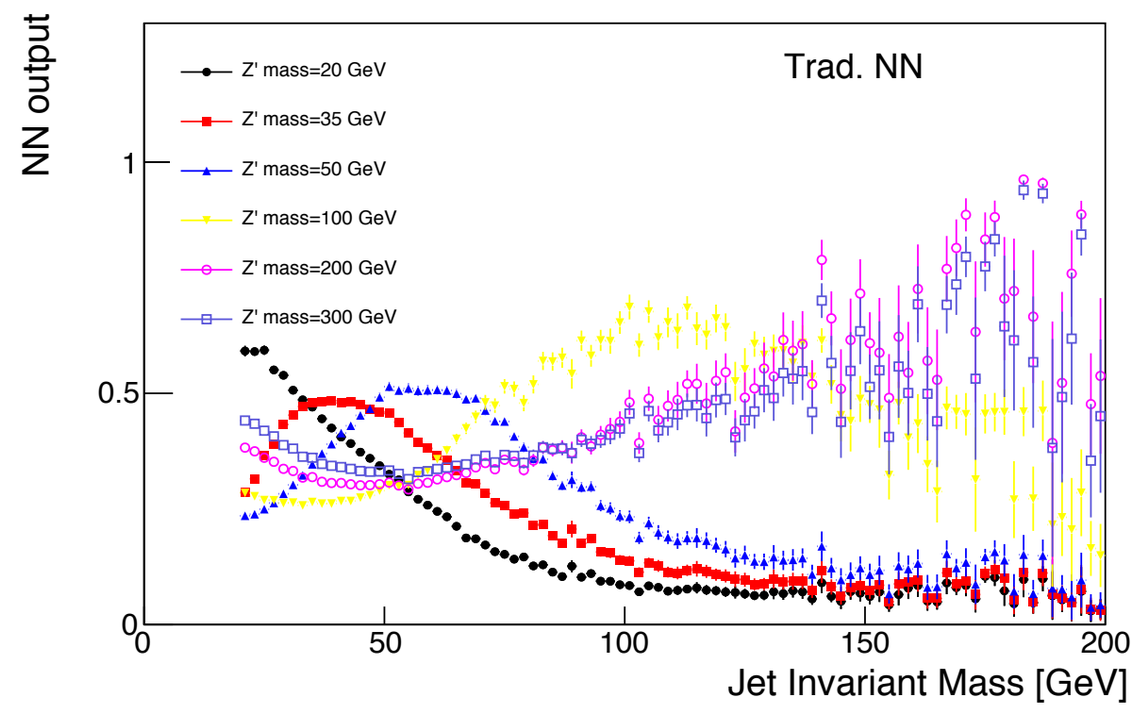
DECORRELATED TAGGERS

K.C, J. Pavez, and G. Louppe, arXiv:1506.02169
P. Baldi, K.C, T. Faucett, P. Sadowski, D. Whiteson arXiv:1601.07913
G. Louppe, M. Kagan, K.C, arXiv:1611.01046
Shimmin, et. al. arXiv:1703.03507

Adversarial approach of "Learning to Pivot" can also be used to train a classifier that is "decorrelated" to some other variable.

- want jet taggers that are decorrelated with jet invariant mass
- so that analysis can still search for a bump using jet invariant mass
- avoids sculpting background





From Reproducibility
To Reusability

[work with Lukas Heinrich]

REINTERPRETATION

The BSM-AI project: SUSY-AI – generalizing LHC limits on supersymmetry with machine learning

Sascha Caron,[a,b] **Jong Soo Kim,**[c] **Krzysztof Rolbiecki,**[c,d]
Roberto Ruiz de Austri,[e] **Bob Stienen**[a]

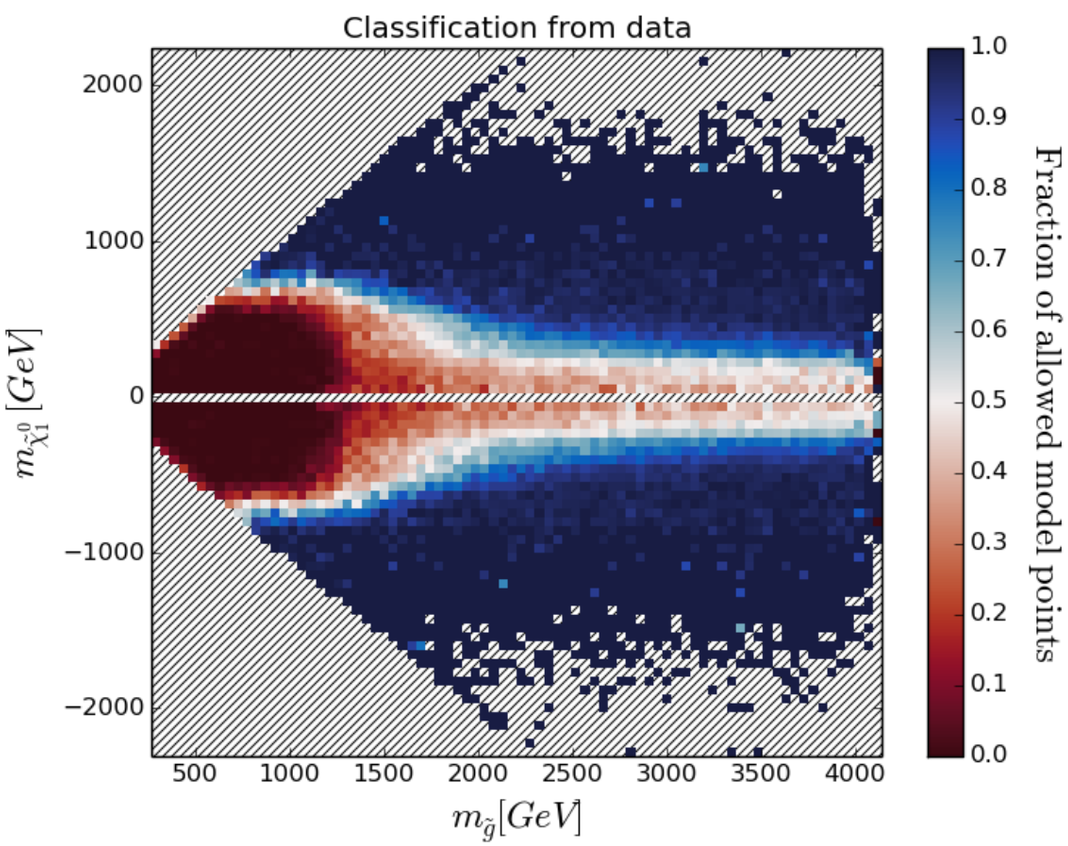
[a] *Institute for Mathematics, Astro- and Particle Physics IMAPP, Radboud Universiteit, Nijmegen, The Netherlands*

[b] *Nikhef, Amsterdam, The Netherlands*

[c] *Instituto de Física Teórica UAM/CSIC, Madrid, Spain*

[d] *Faculty of Physics, University of Warsaw, Warsaw, Poland*

[e] *Instituto de Física Corpuscular, IFIC-UV/CSIC, Valencia, Spain*



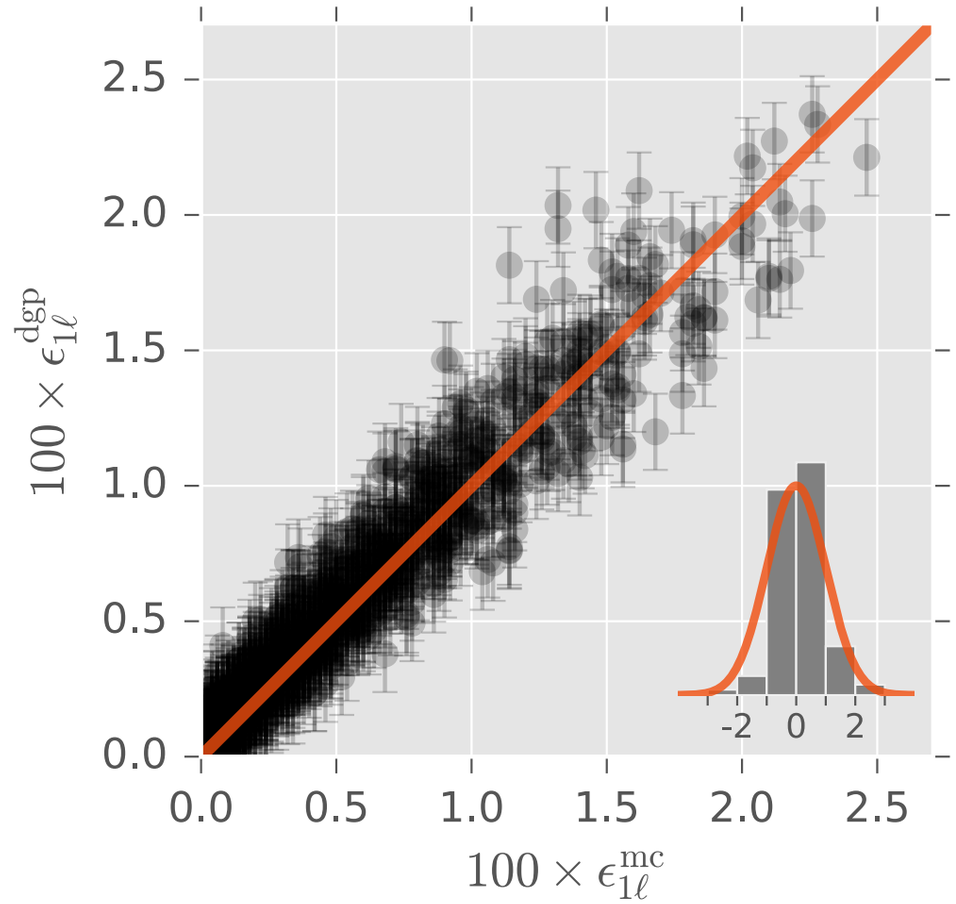
Accelerating the BSM interpretation of LHC data with machine learning

Gianfranco Bertone,[1] Marc Peter Deisenroth,[2] Jong Soo Kim,[3]
Sebastian Liem,[1] Roberto Ruiz de Austri,[4] and Max Welling[5]

[1] *GRAPPA, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands*
[2] *Department of Computing, Imperial College London, 180 Queen's Gate, SW7 2AZ London, United Kingdom*
[3] *Center for Theoretical Physics of the Universe, Institute for Basic Science (IBS), Daejeon, 34051, Korea and Instituto de Física Teórica UAM/CSIC, Madrid, Spain*
[4] *Instituto de Física Corpuscular IFIC-UV/CSIC, Valencia, Spain*
[5] *Informatics Institute, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands*

(Dated: November 10, 2016)

The interpretation of Large Hadron Collider (LHC) data in the framework of Beyond the Standard Model (BSM) theories is hampered by the need to run computationally expensive event generators and detector simulators. Performing statistically convergent scans of high-dimensional BSM theories is consequently challenging, and in practice unfeasible for very high-dimensional BSM theories. We present here a new machine learning method that accelerates the interpretation of LHC data, by learning the relationship between BSM theory parameters and data. As a proof-of-concept, we demonstrate that this technique accurately predicts natural SUSY signal events in two signal regions at the High Luminosity LHC, up to four orders of magnitude faster than standard techniques. The new approach makes it possible to rapidly and accurately reconstruct the theory parameters of complex BSM theories, should an excess in the data be discovered at the LHC.



It’s the difference between if you had airplanes where you threw away an airplane after every flight, versus you could reuse them multiple times.

— Elon Musk

analysis pipeline

analyses pipeline

testing

one theory

It's the difference between if you had ~~airplanes~~ ~~airplane~~ where you threw away an ~~airplane~~ after ~~every flight~~, versus you could reuse them multiple times.

— Elon Musk

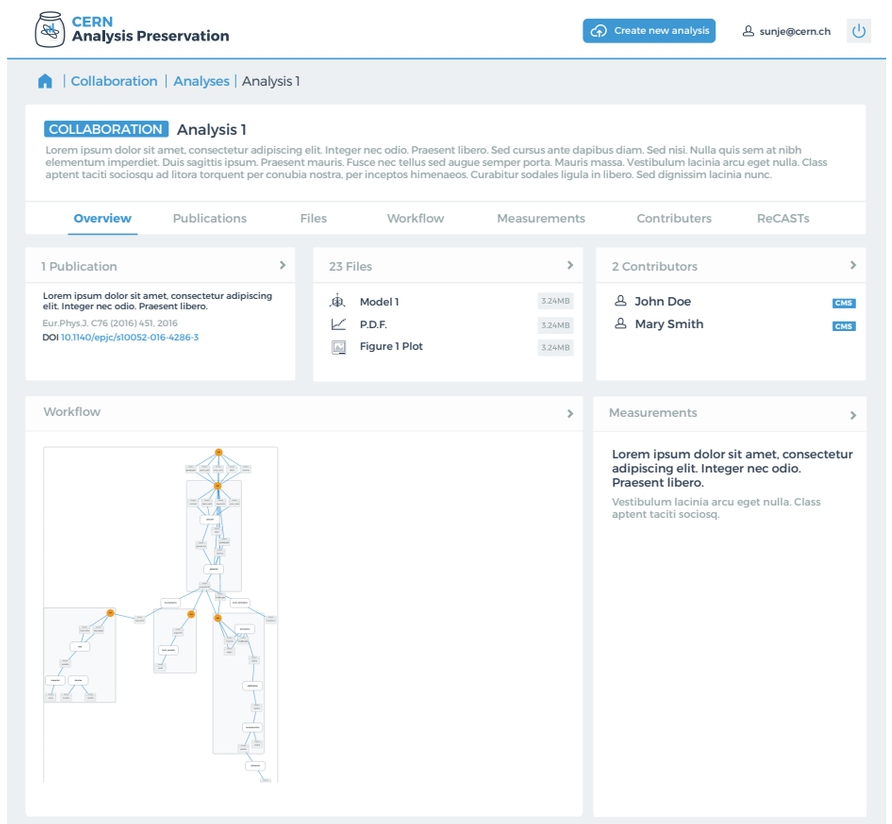
Technical Solution:

Workflow (i.e. logic which steps to run in which order: reconstruction → analysis→ fit)

- in easy to write / read text based format (YAML)
- generic workflow language “**yadage**” based on graphs. No assumption on how you run your analysis. Should be able to accommodate your workflows.
- integrated into CERN Analysis Preservation.
- re-run workflow using tool that interprets info stored in CAP

workflow	software	data
`eventsel.yml`	`docker img`	`data, bkgds`
`fit.yml`	`docker img`	
`workflow.yml`		

import analysis workflow



https://arxiv.org/pdf/1706.01878.pdf

CERN Analysis Preservation

SOFTWARE

Yadage and Packtivity – analysis preservation using parametrized workflows

Kyle Cranmer[1] **and Lukas Heinrich**[1]

[1] Department of Physics, New York University, New York, USA

E-mail: `lukas.heinrich@cern.ch`

Abstract. Preserving data analyses produced by the collaborations at LHC in a parametrized fashion is crucial in order to maintain reproducibility and re-usability. We argue for a declarative description in terms of individual processing steps – "packtivities" – linked through a dynamic directed acyclic graph (DAG) and present an initial set of JSON schemas for such a description and an implementation – "yadage" – capable of executing workflows of analysis preserved via Linux containers.

GitHub, Inc.

yadage - yaml based adage

DOI 10.5281/zenodo.309288 | pypi package 0.10.8 | build passing | health 94% | coverage 90% | docs latest | version git-master

A declarative way to define adage workflows using a JSON schema (but we'll always write it as YAML)

```
docker run --rm -it -v /var/run/docker.sock:/var/run/docker.sock -v $PWD:$PWD -w $PWD lukasheinrich/yada
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

or just

```
eval "$(curl https://raw.githubusercontent.com/diana-hep/yadage/master/yadagedocker.sh)"
yadage-run -t from-github/phenochain mdwork madgraph_delphes.yml -p nevents=100
```

This package reads and executes workflows adhering to the workflow JSON schemas defined at https://github.com/diana-hep/cap-schemas such as the onces stored in the community repository https://github.com/lukasheinrich/yadage-workflows. For executing the individual steps it mainly uses the packtivity python bindings provided by https://github.com/diana-hep/packtivity.

Possible Backends:

Yadage can run on various backends such as multiprocessing pools, ipython clusters, or celery clusters. If human intervention is needed for certain steps, it can also be run interactively.

Example Workflow

```
stages:
  - name: hello_world
```

reana.readthedocs.io

Fork me on GitHub

REANA - Reusable Analyses

build passing | coverage 100% | docs latest | Issues ready for work 2 | gitter join chat | license GNU General Public License v2.0

REANA is a system that permits to instantiate research data analyses on the cloud. It uses container-based technologies and was born to target the use case of particle physics analyses in LHC collaborations. The system paves the way to reusing and reinterpreting preserved data analyses even several years after the original analysis.

REANA - Reusable Analyses

Navigation

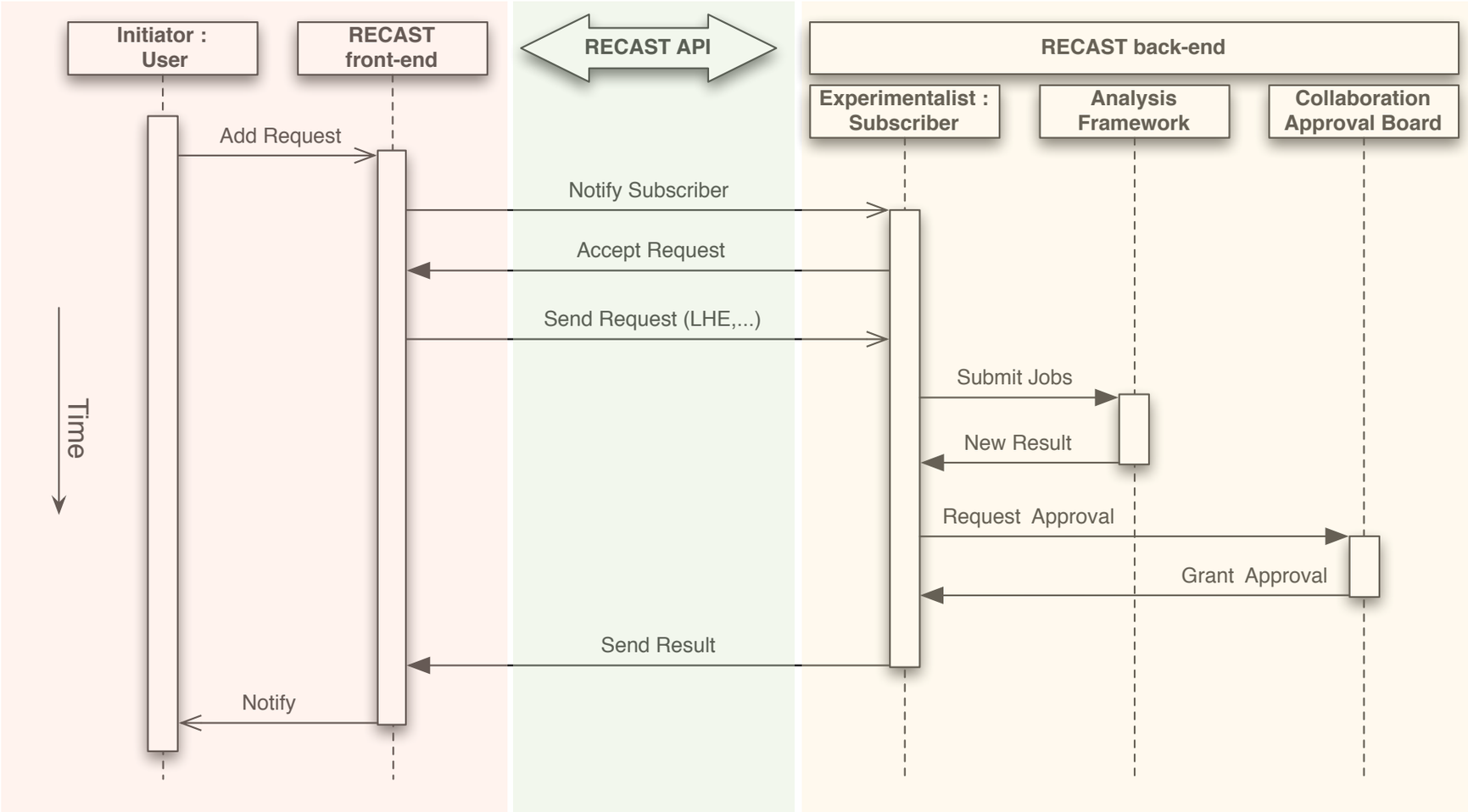
REANA@DockerHub
REANA@GitHub

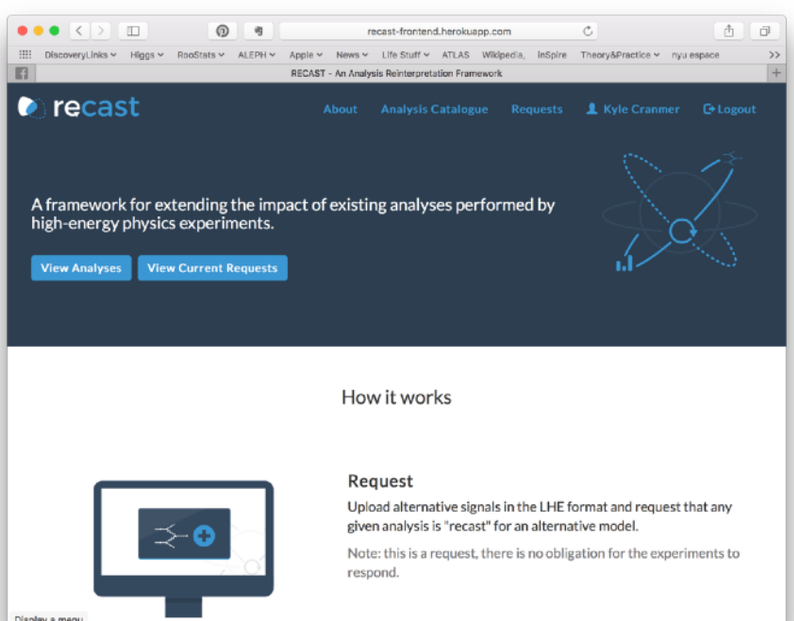
Quick search

Go

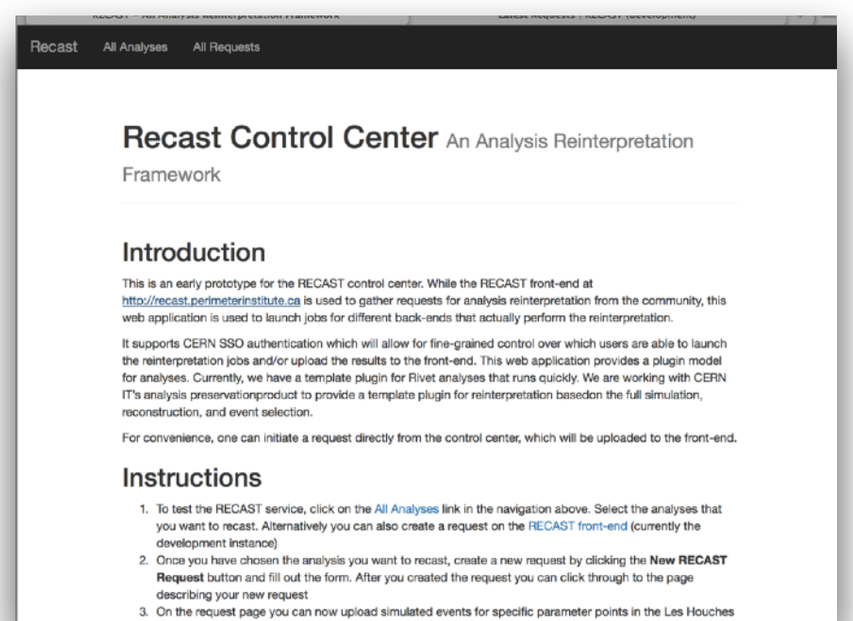
v: latest

https://arxiv.org/pdf/1706.01878.pdf

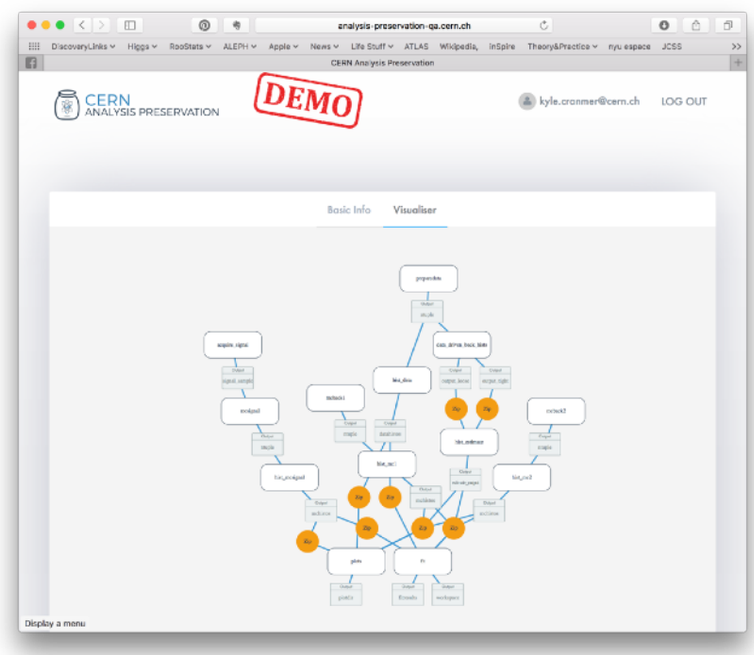




Front-End: public facing
collects requests



Control Center: not public, uses CERN auth.,
oversees processing of jobs on back-end



CERN Analysis Preservation:
Stores workflows, provides back-end
computing resources

Putting it all together

https://github.com/cranmer/active_sciencing

SYNTHESIS

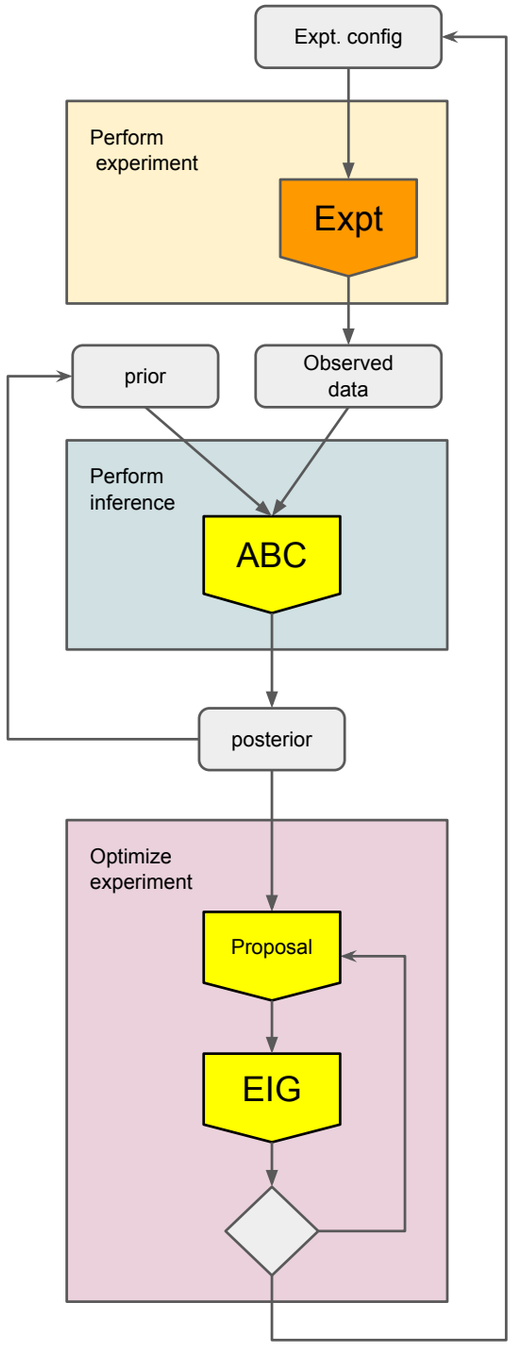
active learning / sequential design / black box optimization

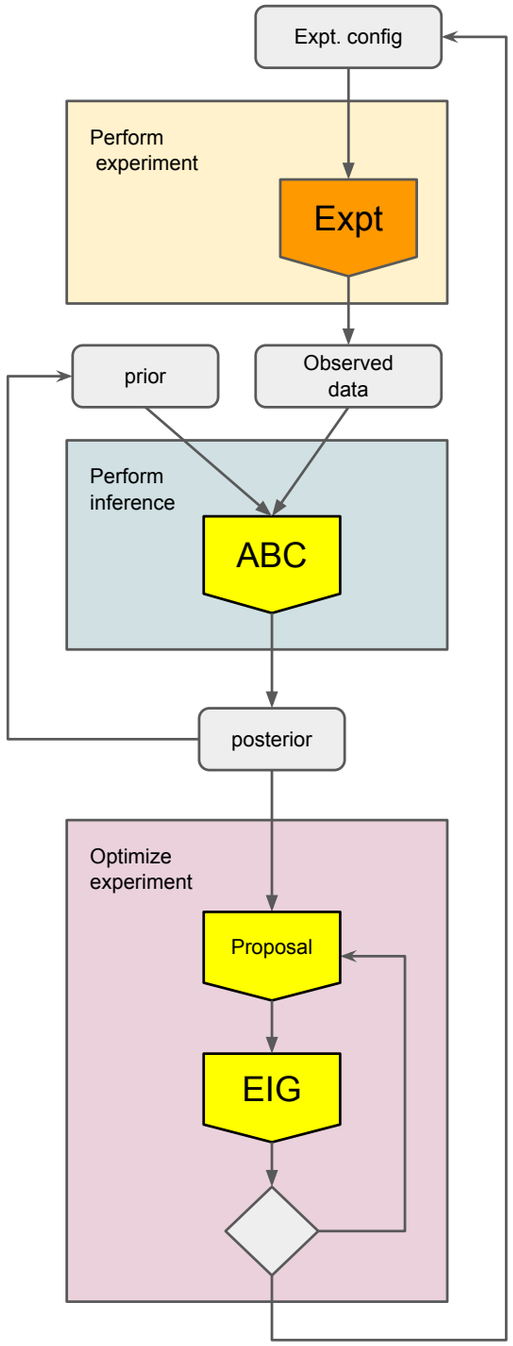
Active Sciencing

reusable workflows

simulation-based
inference engines

https://github.com/cranmer/active_sciencing


Expt. config
Perform experiment
Expt
prior
Observed data
Perform inference
ABC
posterior
Optimize experiment
Proposal
EIG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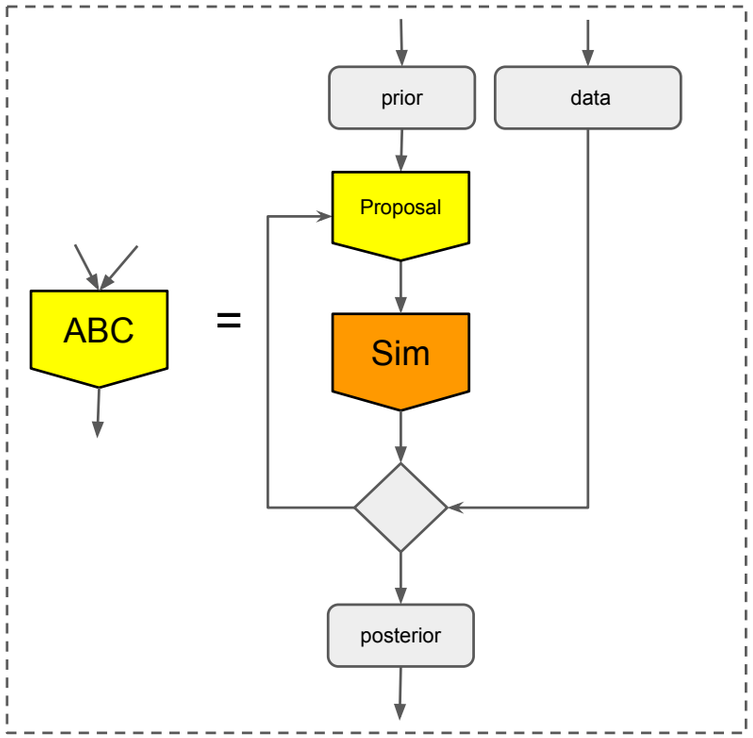
ABC
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data
Proposal
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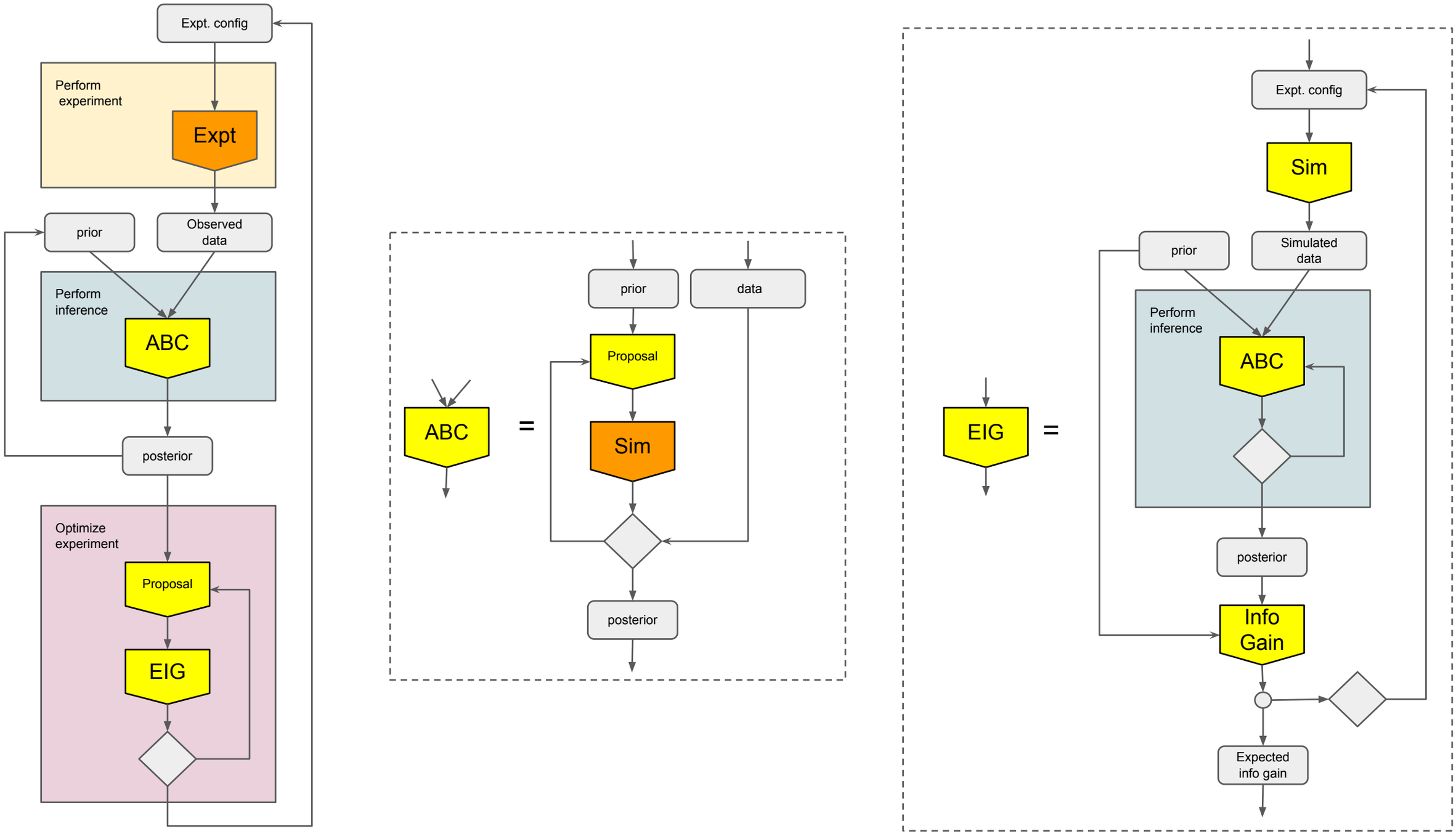
posterior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posterior
EIG
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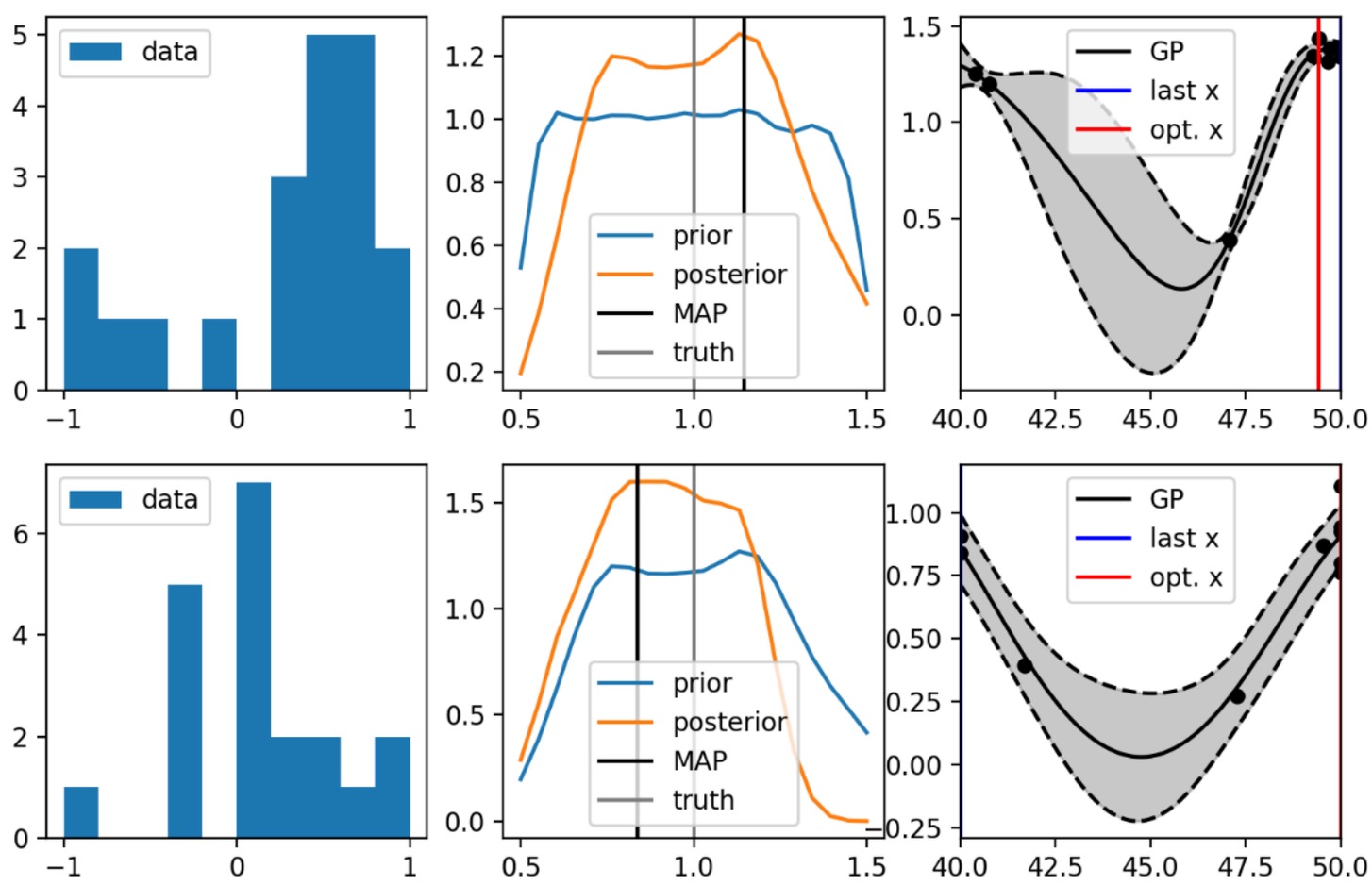
Expt. config
Sim
prior
Simulated data
Perform inference
ABC
posterior
Info Gain
Expected info gain

ACTIVE SCIENCING DEMO

Input:

- workflow for performing "real" experiment that returns data
- workflow for running simulator given parameters of theory and experimental configuration

Demo shows use of likelihood-free inference technique & Bayesian Optimization to measure the Weinberg angle and optimize beam energy (eg. just above or below $M_Z/2$)



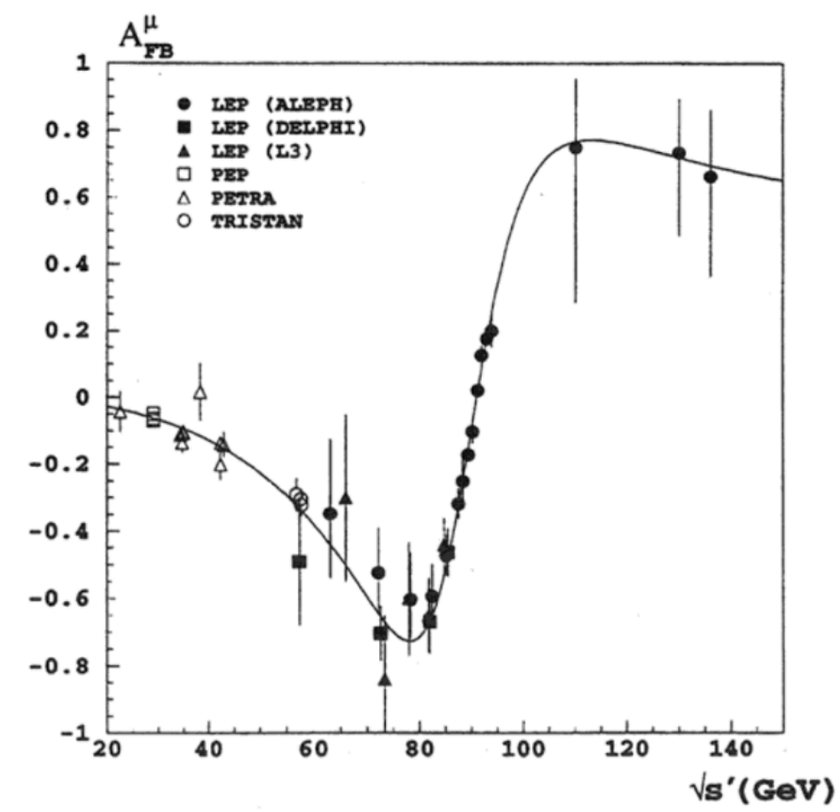


Figure 2: Measured forward-backward asymmetries of muon-pair production compared with the model independent fit results.

ENCAPSULATING THE SIMULATION

https://github.com/lukasheinrich/weinberg-test

README.md

Run HEP workflows from the web.

by Kyle Cranmer and Lukas Heinrich

An example notebook on how to generate simulated high energy physics collision events using the generator package MadGraph. Simulated datasets obtained from this notebook can then be used to train and evaluate the performance of generative models for physics.

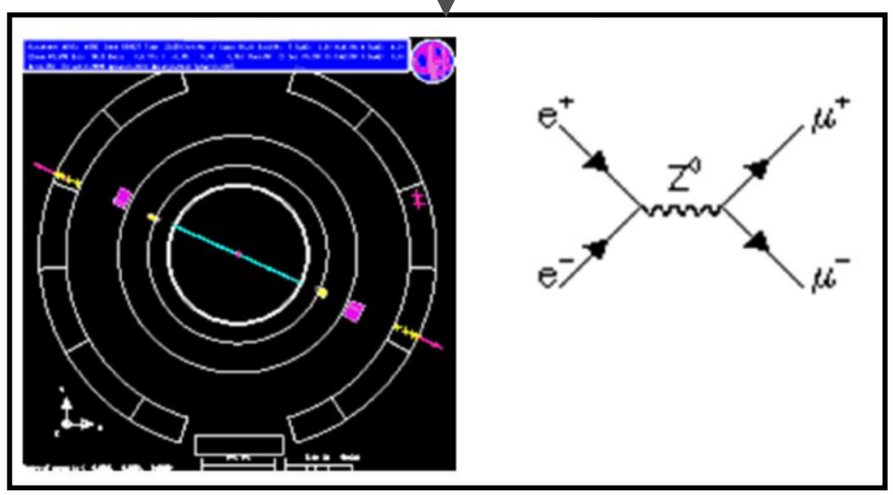
Usage:

This repository has been equipped with a Dockerfile to encapsulate its software environment. It can be used with the mybinder service to launch an ephemeral jupyter notebook server to run the notebook.

Click on the below badge and open the notebook `adage.ipynb`.

launch binder

$$
\begin{aligned}
\mathcal{L}_{SM} = \quad & \underbrace{\frac{1}{4}\mathbf{W}_{\mu\nu}\cdot\mathbf{W}^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\
& + \underbrace{\bar{L}\gamma^\mu(i\partial_\mu - \frac{1}{2}g\tau\cdot\mathbf{W}_\mu - \frac{1}{2}g'YB_\mu)L \;+\; \bar{R}\gamma^\mu(i\partial_\mu - \frac{1}{2}g'YB_\mu)R}_{\text{kinetic energies and electroweak interactions of fermions}} \\
& + \underbrace{\frac{1}{2}\left|(i\partial_\mu - \frac{1}{2}g\tau\cdot\mathbf{W}_\mu - \frac{1}{2}g'YB_\mu)\,\phi\right|^2 - V(\phi)}_{W^\pm, Z, \gamma, \text{and Higgs masses and couplings}} \\
& + \underbrace{g''(\bar{q}\gamma^\mu T_a q)\,G^a_\mu}_{\text{interactions between quarks and gluons}} \quad + \underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\text{fermion masses and couplings to Higgs}}
\end{aligned}
$$



other electroweak parameters. This can be shown with Eq. (2.96), giving

$$
A^f_{FB}(s) \simeq A^f_{FB}(m_Z^2) + \frac{(s - m_Z^2)}{s}\,\frac{3\pi\alpha(s)}{\sqrt{2}G_F m_Z^2}\,\frac{2Q_e Q_f g_{Ae} g_{Af}}{(g^2_{Ve} + g^2_{Ae})(g^2_{Vf} + g^2_{Af})} \;. \quad (8.30)
$$

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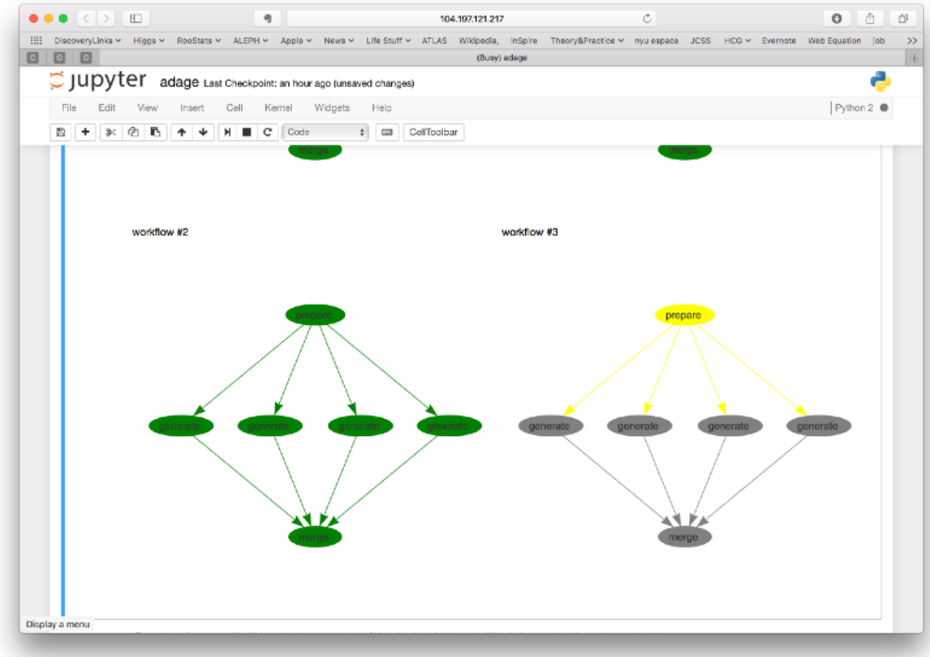
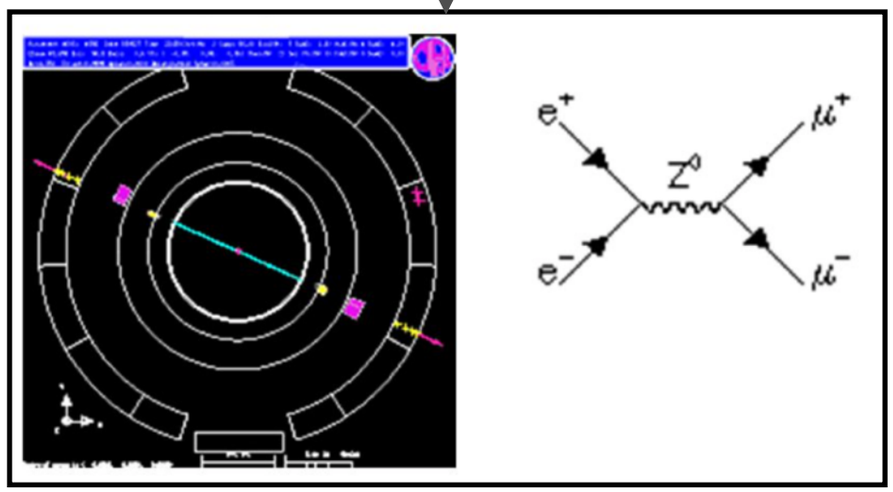


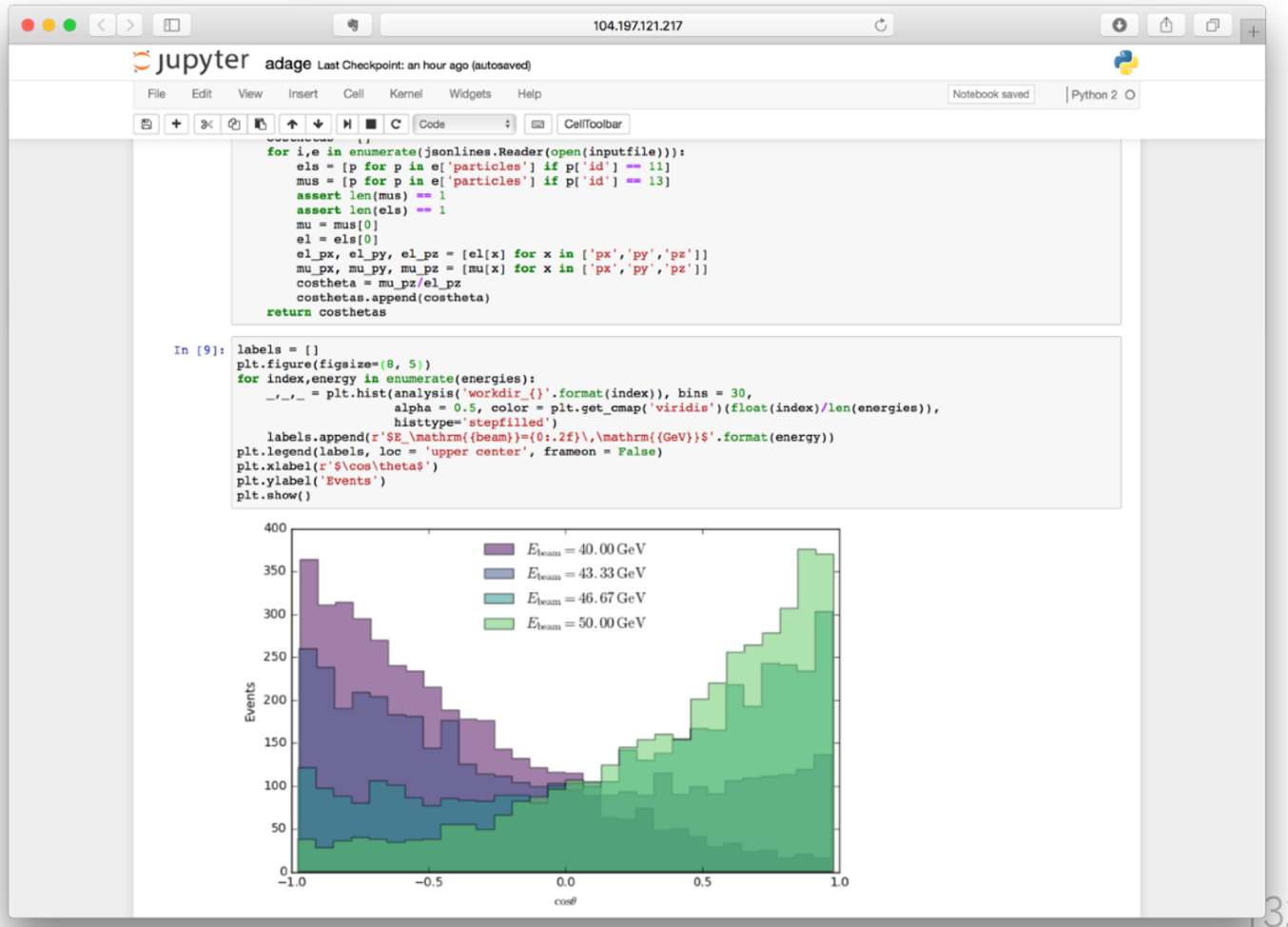
$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4}\mathbf{W}_{\mu\nu}\cdot\mathbf{W}^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}}$$

$$+ \underbrace{\bar{L}\gamma^\mu(i\partial_\mu - \frac{1}{2}g\tau\cdot\mathbf{W}_\mu - \frac{1}{2}g'YB_\mu)L + \bar{R}\gamma^\mu(i\partial_\mu - \frac{1}{2}g'YB_\mu)R}_{\text{kinetic energies and electroweak interactions of fermions}}$$

$$+ \underbrace{\frac{1}{2}\left|(i\partial_\mu - \frac{1}{2}g\tau\cdot\mathbf{W}_\mu - \frac{1}{2}g'YB_\mu)\,\phi\right|^2 - V(\phi)}_{W^\pm, Z, \gamma, \text{and Higgs masses and couplings}}$$

$$+ \underbrace{g''(\bar{q}\gamma^\mu T_a q)\,G^a_\mu}_{\text{interactions between quarks and gluons}} + \underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\text{fermion masses and couplings to Higgs}}$$

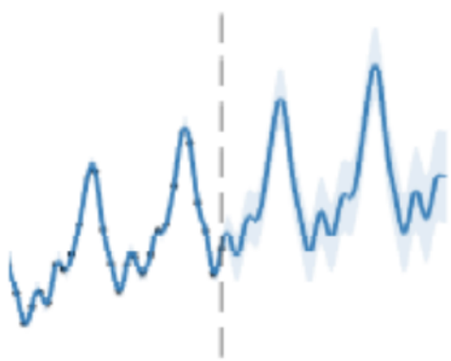




SEARCHING OVER SPACE OF MODELS

Vocabulary of kernels + grammar for composition

- physics goes into the construction of a "Kernel" that describes covariance of data

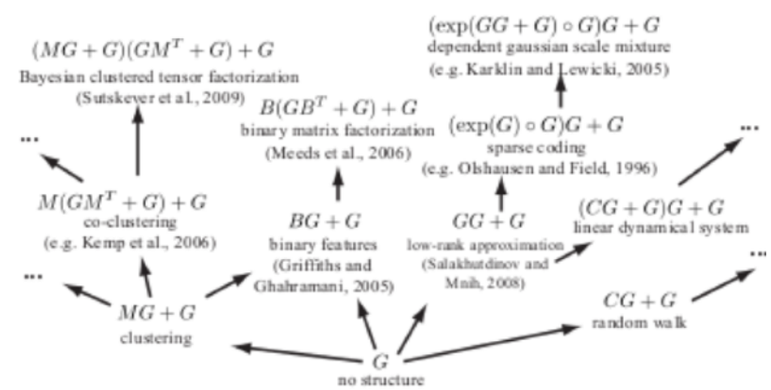


Structure Discovery in Nonparametric Regression through Compositional Kernel Search

David Duvenaud, James Robert Lloyd, Roger Grosse, Joshua B. Tenenbaum, Zoubin Ghahramani

International Conference on Machine Learning, 2013

pdf | code | poster | bibtex



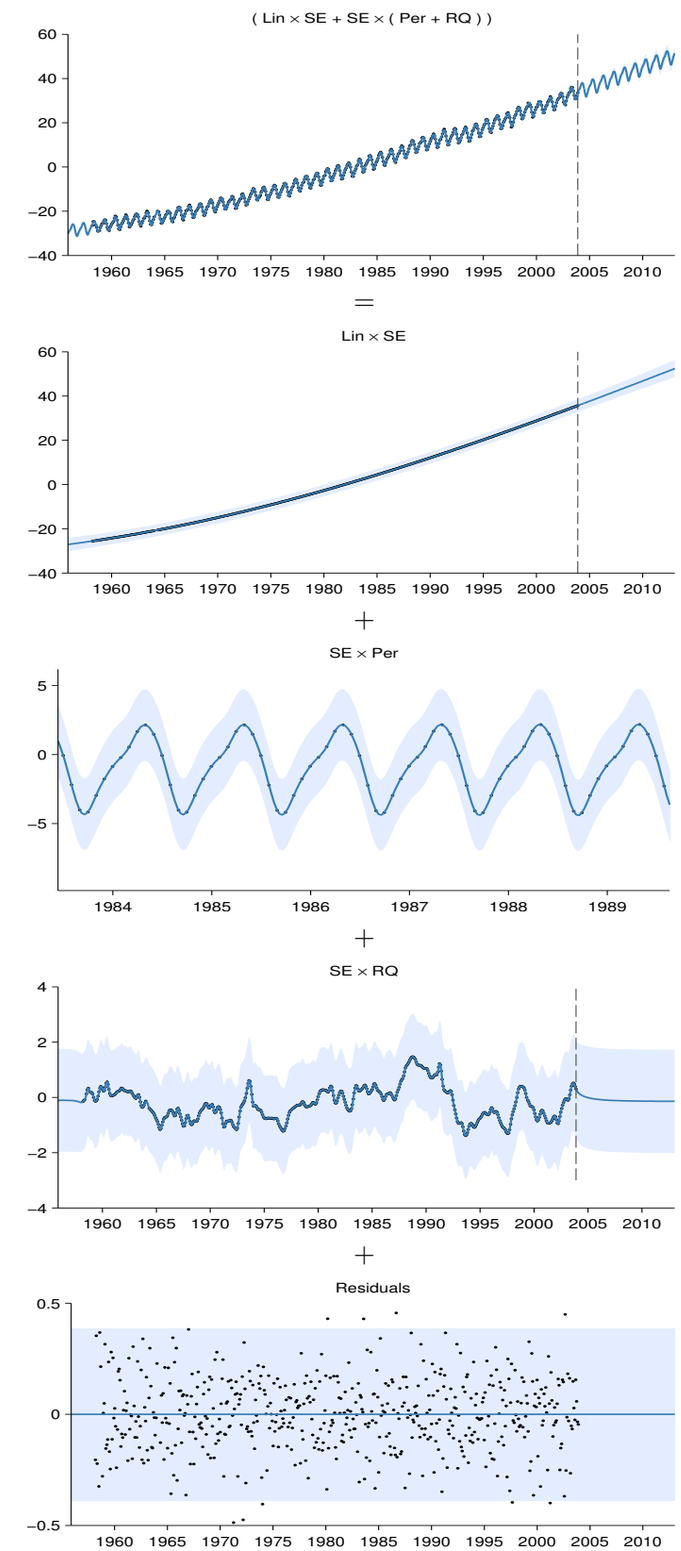
Exploiting compositionality to explore a large space of model structures

Roger Grosse, Ruslan Salakhutdinov, William T. Freeman, Joshua B. Tenenbaum

Conference on Uncertainty in Artificial Intelligence, 2012

pdf | code | bibtex

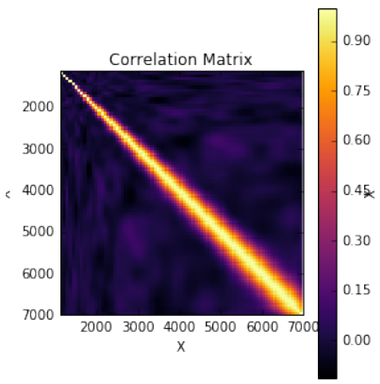
Mauna Loa atmospheric CO_2



GAUSSIAN PROCESSES AT LHC

with Meghan Frate

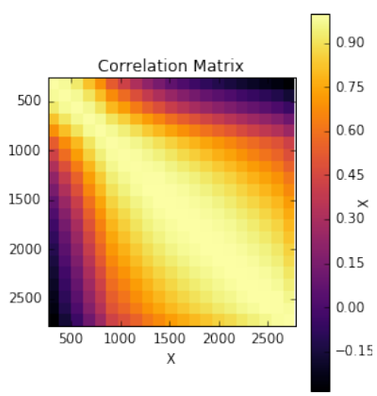
Instead of fitting the dijet spectrum with an ad hoc 3-5 parameter function, use GP with kernel motivated from physics



Final Kernel =

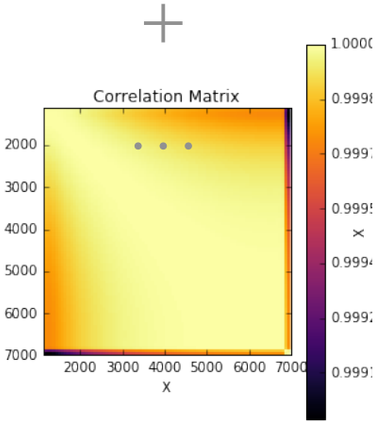
Poisson stats
+ Mass Resolution

=



+ Parton Density Functions

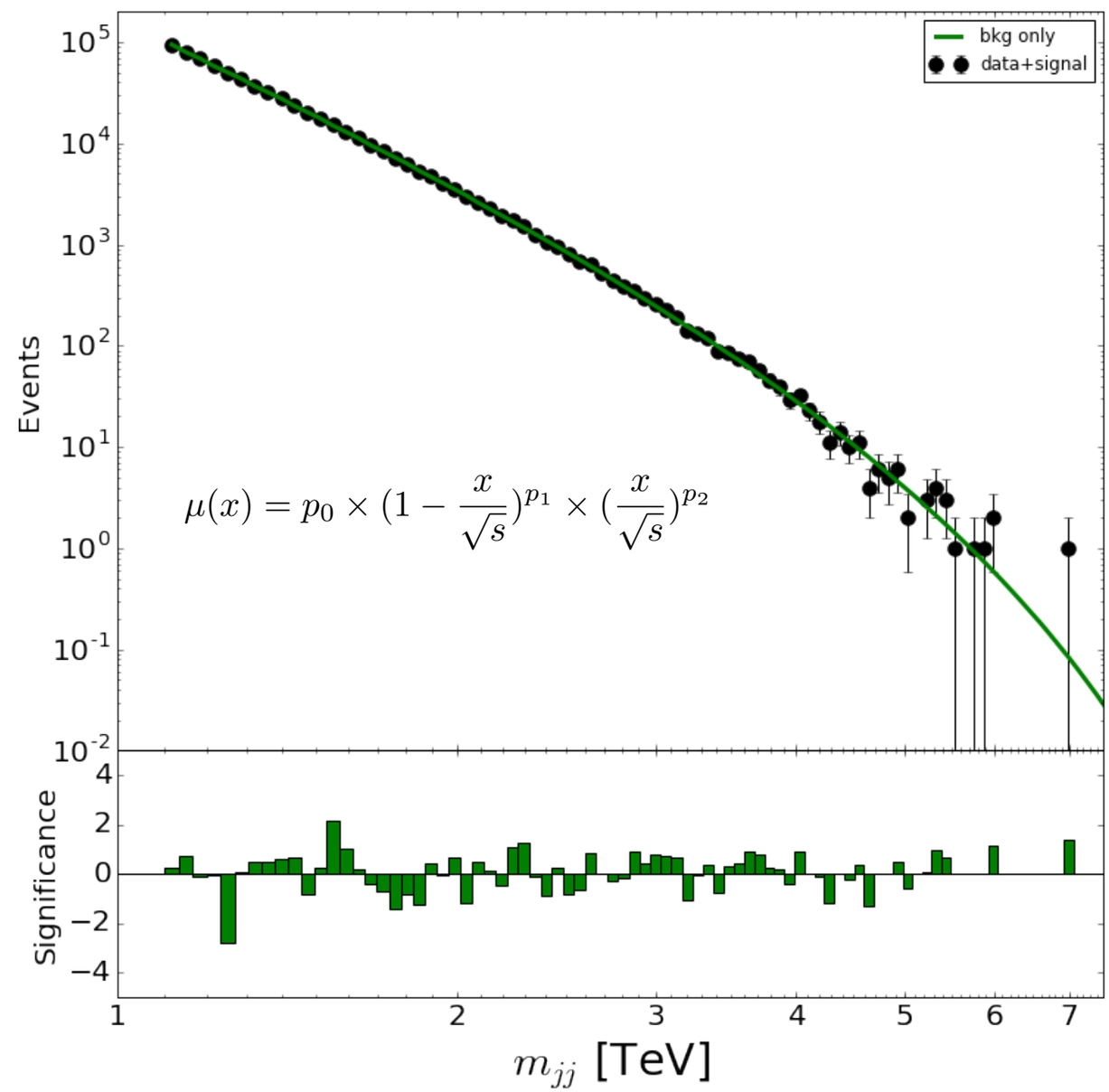
+



+ Jet Energy Scale

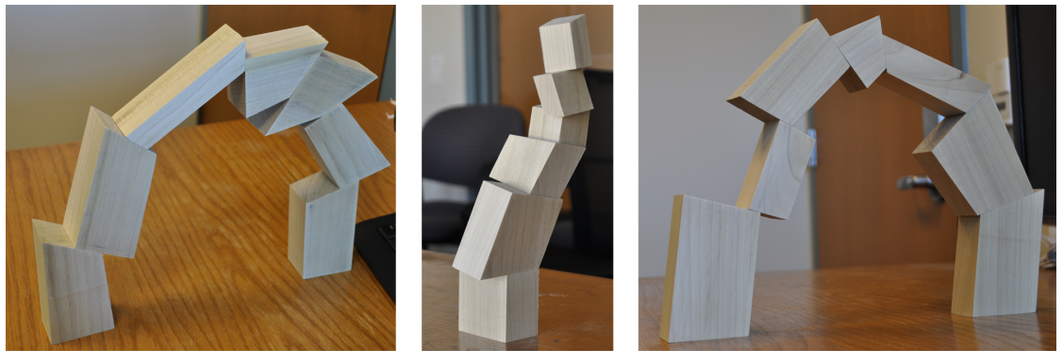
+

. . .

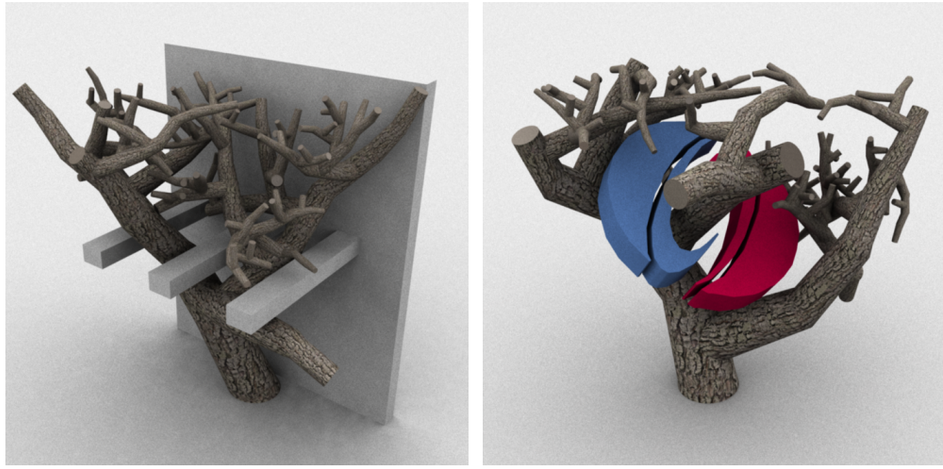


Directed Procedural Graphics

Stable Static Structures



Procedural Graphics



$\mathbf{x}$	$\mathbf{y}$
simulation	constraint

Ritchie, Lin, Goodman, & Hanrahan.
Generating Design Suggestions under Tight Constraints
with Gradient-based Probabilistic Programming.
In Computer Graphics Forum, (2015)

Ritchie, Mildenhall, Goodman, & Hanrahan.
"Controlling Procedural Modeling Programs with
Stochastically-Ordered Sequential Monte Carlo."
SIGGRAPH (2015)

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THANKS!

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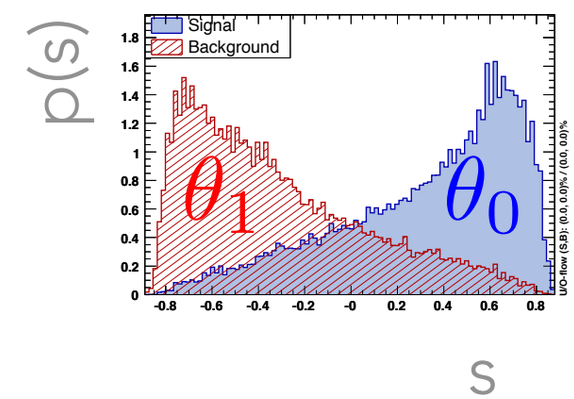
CARL

The intractable likelihood ratio based on high-dimensional features x is:

$$\frac{p(x|\theta_0)}{p(x|\theta_1)}$$

We can show that an **equivalent test** can be made from 1-D projection

$$\frac{p(x|\theta_0)}{p(x|\theta_1)} = \frac{p(s(x;\theta_0,\theta_1)|\theta_0)}{p(s(x;\theta_0,\theta_1)|\theta_1)}$$



if the scalar map s: X → $\mathbb{R}$ has the same level sets as the likelihood ratio

$$s(x;\theta_0;\theta_1) = \text{monotonic}[\ p(x|\theta_0)/p(x|\theta_1)\ ]$$

Estimating the density of $s(x;\theta_0,\theta_1)$ via the simulator calibrates the ratio.

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

Binary classifier on balanced y=0 and y=1 labels learns

$$s(x) = \frac{p(x|y=1)}{p(x|y=0) + p(x|y=1)}$$

Which is one-to-one with the likelihood ratio

$$\frac{p(x|y=0)}{p(x|y=1)} = 1 - \frac{1}{s(x)}$$

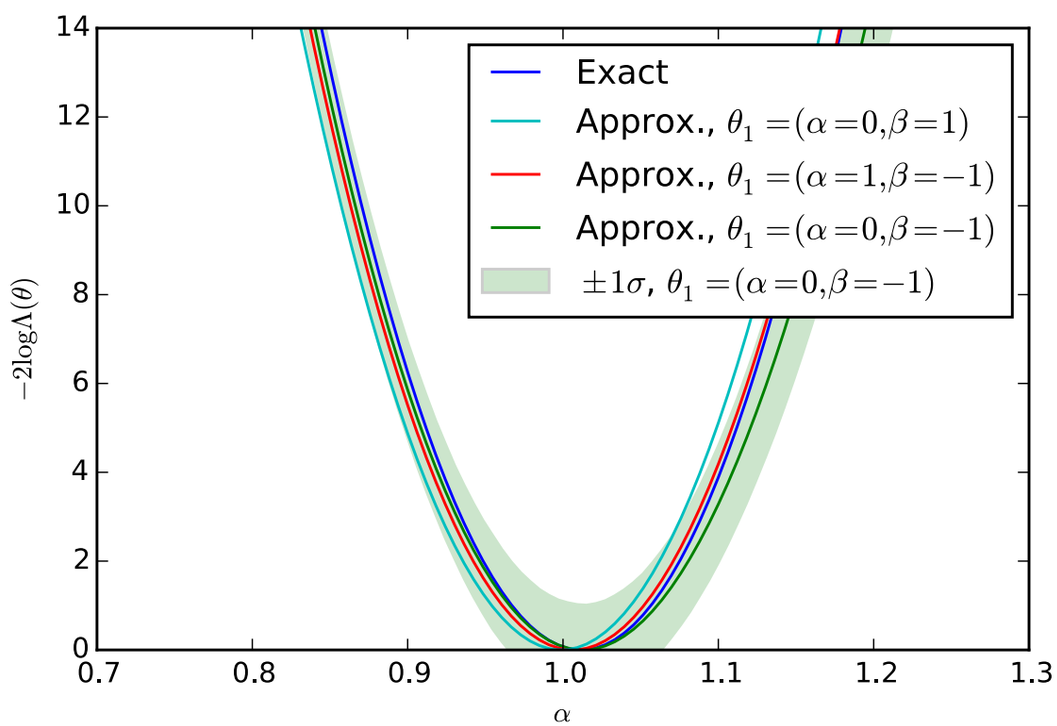
Can do the same thing for any two points θ_0 & θ_1 in parameter space. I call this a **parametrized classifier**

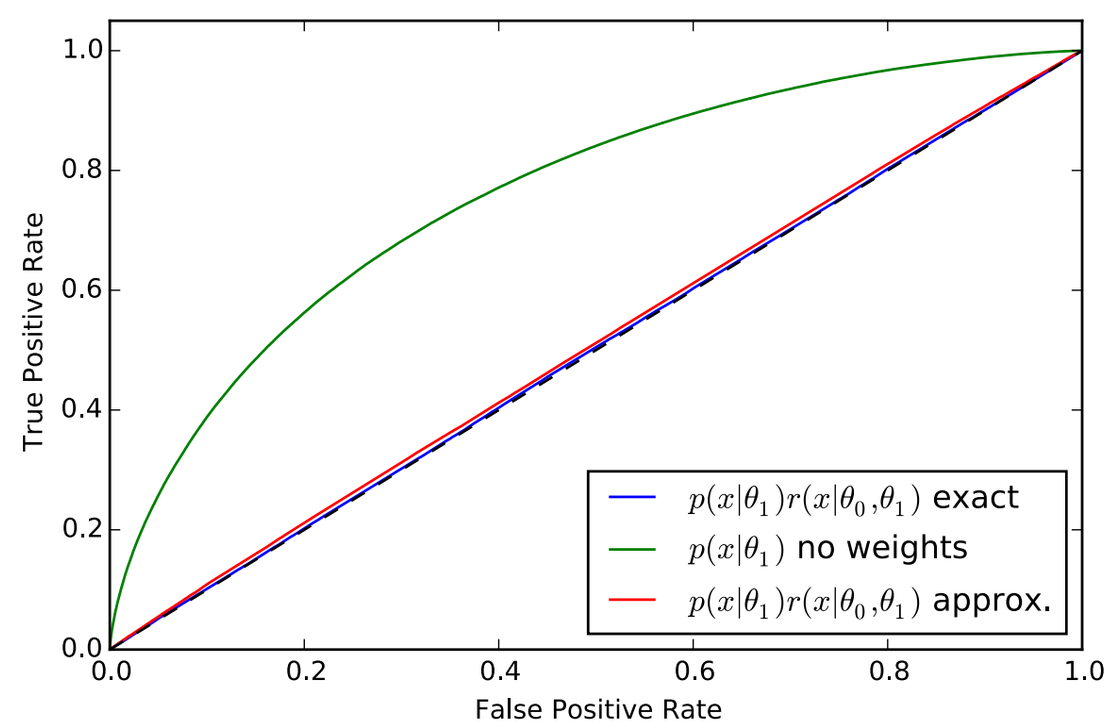
$$s(x; \theta_0, \theta_1) = \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}$$

DIAGNOSTICS

In practice $\hat{r}(\hat{s}(\mathbf{x};\theta_0,\theta_1))$ will not be exact. Diagnostic procedures are needed to assess the quality of this approximation.

1. For inference, the value of the MLE $\hat{\theta}$ should be independent of the value of θ_1 used in the denominator of the ratio.
2. Train a classifier to distinguish between unweighted samples from $p(\mathbf{x}|\theta_0)$ and samples from $p(\mathbf{x}|\theta_1)$ weighted by $\hat{r}(\hat{s}(\mathbf{x};\theta_0,\theta_1))$.





$$\frac{p_1(s^*)}{p_0(s^*)} = \frac{p_1(x)}{p_0(x)} \boxed{\frac{\int d\Omega_{s^*} p_0(x)/|\hat{n}\cdot\nabla s|}{\int d\Omega_{s^*} p_0(x)/|\hat{n}\cdot\nabla s|}} = \frac{p_1(x)}{p_0(x)}$$