Approximating likelihood ratios with calibrated classifiers

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Joint work with

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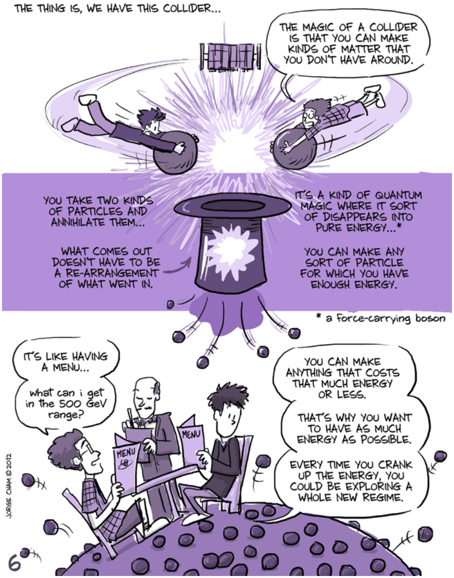
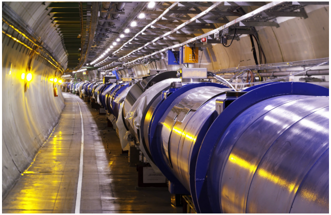
See paper (Cranmer et al., 2015) for full details.

Studying the constituents of the universe





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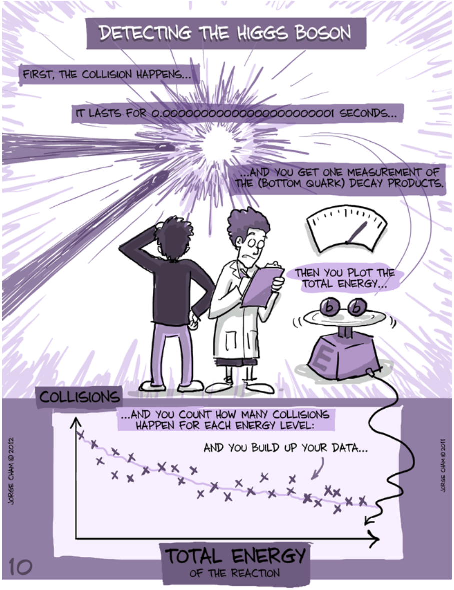
Collecting data



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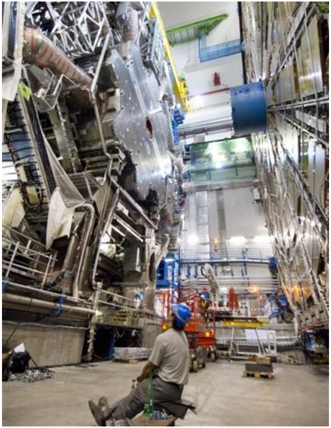
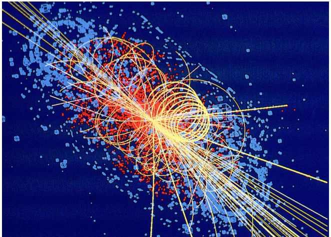
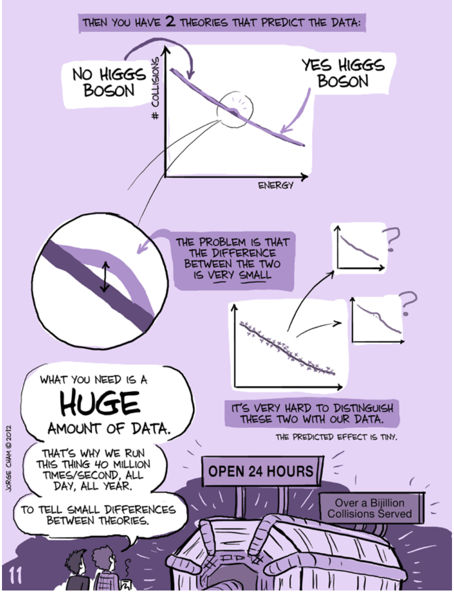




Testing for new physics



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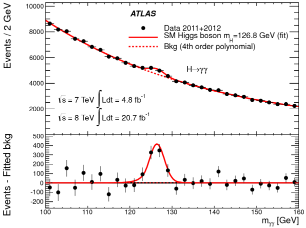
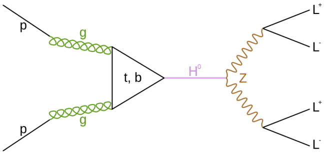


$$\frac{p(\text{data}|\text{theory} + X)}{p(\text{data}|\text{theory})}$$

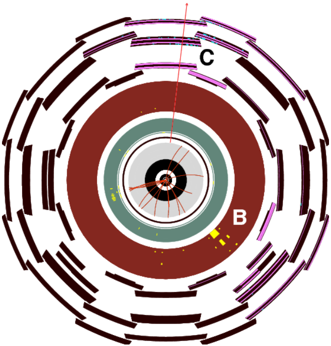
Likelihood-free setup

- Complex simulator p parameterized by θ;
- Samples $\mathbf{x} \sim p$ can be generated on-demand;
- ... but the likelihood $p(\mathbf{x}|\theta)$ cannot be evaluated!

$p =$



$\otimes$



Simple hypothesis testing

- Assume some observed data $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$;
- Test a null $\theta = \theta_0$ against an alternative $\theta = \theta_1$;
- The Neyman-Pearson lemma states that the most powerful test statistic is

$$\lambda(\mathcal{D}; \theta_0, \theta_1) = \prod_{\mathbf{x} \in \mathcal{D}} \frac{p_{\mathbf{X}}(\mathbf{x}|\theta_0)}{p_{\mathbf{X}}(\mathbf{x}|\theta_1)}.$$

- ... but neither $p_{\mathbf{X}}(\mathbf{x}|\theta_0)$ nor $p_{\mathbf{X}}(\mathbf{x}|\theta_1)$ can be evaluated!

Straight approximation

1. Approximate $p_{\mathbf{X}}(\mathbf{x}|\theta_0)$ and $p_{\mathbf{X}}(\mathbf{x}|\theta_1)$ individually, using density estimation algorithms;
2. Evaluate their ratio $r(\mathbf{x}; \theta_0, \theta_1)$.

Works fine for low-dimensional data, but because of the curse of dimensionality, this is in general a difficult problem! Moreover, it is not even necessary!

$$\frac{p_{\mathbf{X}}(\mathbf{x}|\theta_0)}{p_{\mathbf{X}}(\mathbf{x}|\theta_1)} = r(\mathbf{x}; \theta_0, \theta_1)$$

When solving a problem of interest, do not solve a more general problem as an intermediate step. – Vladimir Vapnik

Likehood ratio invariance under change of variable

Theorem. The likelihood ratio is invariant under the change of variable $\mathbf{U} = s(\mathbf{X})$, provided $s(\mathbf{x})$ is monotonic with $r(\mathbf{x})$.

$$r(\mathbf{x}) = \frac{p_{\mathbf{X}}(\mathbf{x}|\theta_0)}{p_{\mathbf{X}}(\mathbf{x}|\theta_1)} = \frac{p_{\mathbf{U}}(s(\mathbf{x})|\theta_0)}{p_{\mathbf{U}}(s(\mathbf{x})|\theta_1)}$$

Approximating likelihood ratios with classifiers

- Well, a classifier trained to distinguish $\mathbf{x} \sim p_0$ from $\mathbf{x} \sim p_1$ approximates

$$s^*(\mathbf{x}) = \frac{p_{\mathbf{X}}(\mathbf{x}|\theta_1)}{p_{\mathbf{X}}(\mathbf{x}|\theta_0) + p_{\mathbf{X}}(\mathbf{x}|\theta_1)},$$

  which is monotonic with $r(\mathbf{x})$.
- Estimating $p(s(\mathbf{x})|\theta)$ is now easy, since the change of variable $s(\mathbf{x})$ projects $\mathbf{x}$ in a 1D space, where only the informative content of the ratio is preserved.
  - This can be carried out using density estimation or calibration algorithms (histograms, KDE, isotonic regression, etc).
- Disentangle training from calibration.

Inference and composite hypothesis testing

Approximated likelihood ratios can be used for inference, since

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} p(\mathcal{D}|\theta) \\ &= \arg\max_{\theta} \prod_{\mathbf{x}\in\mathcal{D}} \frac{p(\mathbf{x}|\theta)}{p(\mathbf{x}|\theta_1)} \\ &= \arg\max_{\theta} \prod_{\mathbf{x}\in\mathcal{D}} \frac{p(s(\mathbf{x};\theta,\theta_1)|\theta)}{p(s(\mathbf{x};\theta,\theta_1)|\theta_1)} \qquad (1)\end{aligned}$$

where θ_1 is fixed and $s(\mathbf{x};\theta,\theta_1)$ is a family of classifiers parameterized by (θ,θ_1).

Accordingly, generalized (or profile) likelihood ratio tests can be evaluated in the same way.

Parameterized learning

For inference, we need to build a family $s(\mathbf{x}; \theta, \theta_1)$ of classifiers.

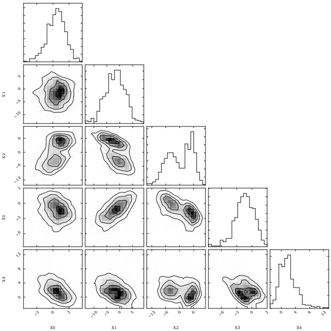
- One could build a classifier s independently for all θ, θ_1. But this is computationally expensive and would not guarantee a smooth evolution of $s(\mathbf{x}; \theta, \theta_1)$ as θ varies.
- Solution: build a single parameterized classifier instead, where parameters are additional input features (Cranmer et al., 2015; Baldi et al., 2016).

$\mathcal{T} := \{\}$;
while size($\mathcal{T}$) $< N$ **do**
  Draw $\theta_0 \sim \pi_{\Theta_0}$;
  Draw $\mathbf{x} \sim p(\mathbf{x}|\theta_0)$;
  $\mathcal{T} := \mathcal{T} \cup \{((\mathbf{x}, \theta_0, \theta_1), y = 0)\}$;
  Draw $\theta_1 \sim \pi_{\Theta_1}$;
  Draw $\mathbf{x} \sim p(\mathbf{x}|\theta_1)$;
  $\mathcal{T} := \mathcal{T} \cup \{((\mathbf{x}, \theta_0, \theta_1), y = 1)\}$;
end while
Learn a single classifier $s(\mathbf{x}; \theta_0, \theta_1)$ from $\mathcal{T}$.

Example: Inference from multidimensional data

Let assume 5D data $\mathbf{x}$ generated from the following process p_0:

1. $\mathbf{z} := (z_0, z_1, z_2, z_3, z_4)$, such that
   $z_0 \sim \mathcal{N}(\mu = \alpha, \sigma = 1)$,
   $z_1 \sim \mathcal{N}(\mu = \beta, \sigma = 3)$,
   $z_2 \sim \text{Mixture}(\frac{1}{2}\mathcal{N}(\mu = -2, \sigma = 1), \frac{1}{2}\mathcal{N}(\mu = 2, \sigma = 0.5))$,
   $z_3 \sim \text{Exponential}(\lambda = 3)$, and
   $z_4 \sim \text{Exponential}(\lambda = 0.5)$;
2. $\mathbf{x} := R\mathbf{z}$, where R is a fixed semi-positive definite 5×5 matrix defining a fixed projection of $\mathbf{z}$ into the observed space.



Observed data $\mathcal{D}$

Our goal is to infer the values α and β based on $\mathcal{D}$.

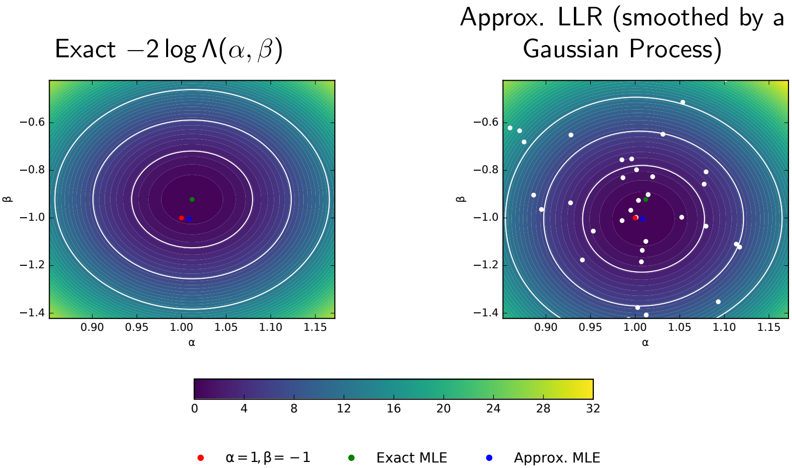
Check out (Louppe et al., 2016) to reproduce this example.

Example: Inference from multidimensional data

Recipe:

1. Build a single parameterized classifier $s(\mathbf{x}; \theta_0, \theta_1)$, in this case a 2-layer NN trained on 5+2 features, with the alternative fixed to $\theta_1 = (\alpha = 0, \beta = 0)$.
2. Find the approximated MLE $\hat{\alpha}, \hat{\beta}$ by solving Eqn. 1.
   - Solve Eqn. 1 using likelihood scans or through optimization.
   - Since the generator is inexpensive, $p(s(\mathbf{x}; \theta_0, \theta_1)|\theta)$ can be calibrated on-the-fly, for every candidate (α, β), e.g. using histograms.
3. Construct the log-likelihood ratio (LLR) statistic

$$-2 \log \Lambda(\alpha, \beta) = -2 \log \frac{p(\mathcal{D}|\alpha, \beta)}{p(\mathcal{D}|\hat{\alpha}, \hat{\beta})}$$

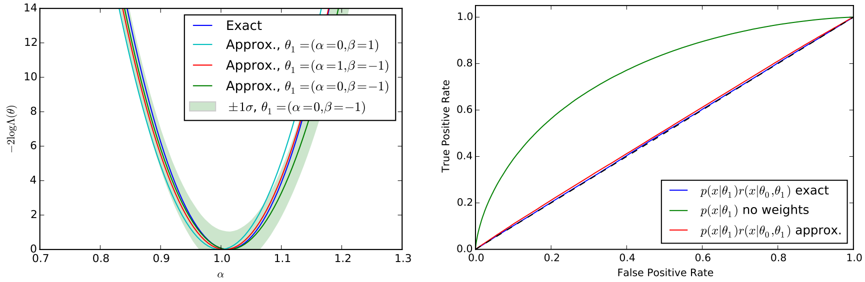


Exact $-2\log\Lambda(\alpha,\beta)$
Approx. LLR (smoothed by a Gaussian Process)
β
α
−0.6
−0.8
−1.0
−1.2
−1.4
0.90
0.95
1.00
1.05
1.10
1.15
0 4 8 12 16 20 24 28 32
$\alpha = 1, \beta = -1$
Exact MLE
Approx. MLE

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 $\hat{r}(\hat{s}(\mathbf{x};\theta_0,\theta_1))$.



Density ratio estimation

Approximating likelihood ratios relates to many other fundamental statistical inference problems, including

- transfer learning,
- outlier detection,
- divergence estimation,
- ...

Transfer learning: $p_{\text{train}} \neq p_{\text{test}}$

As training data increases, i.e. as $N \to \infty$,

$$\frac{1}{N}\sum_{\mathbf{x}_i} L(\varphi(\mathbf{x}_i)) \to \int L(\varphi(\mathbf{x}))p_{\text{train}}(\mathbf{x})d\mathbf{x}.$$

We want to be good on test data, i.e., minimize

$$\int L(\varphi(\mathbf{x}))p_{\text{test}}(\mathbf{x})d\mathbf{x}.$$

Solution: *importance weighting*.

$$\varphi^* = \arg\min_{\varphi} \frac{1}{N}\sum_{\mathbf{x}_i} \frac{p_{\text{test}}(\mathbf{x}_i)}{p_{\text{train}}(\mathbf{x}_i)} L(\varphi(\mathbf{x}_i))$$

Summary

- We proposed an approach for approximating LR in the likelihood-free setup.
- Evaluating likelihood ratios reduces to supervised learning. Both problems are deeply connected.
- Alternative to Approximate Bayesian Computation, without the need to define a prior over parameters.

References

Baldi, P., Cranmer, K., Faucett, T., Sadowski, P., and Whiteson, D. (2016). Parameterized Machine Learning for High-Energy Physics. *arXiv preprint arXiv:1601.07913*.

Cranmer, K., Pavez, J., and Louppe, G. (2015). Approximating likelihood ratios with calibrated discriminative classifiers. *arXiv preprint arXiv:1506.02169*.

Louppe, G., Cranmer, K., and Pavez, J. (2016). carl: a likelihood-free inference toolbox. `http://dx.doi.org/10.5281/zenodo.47798`, `https://github.com/diana-hep/carl`.