Machine Learning Techniques at the LHC Experiments

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DE LA RECHERCHE À L'INDUSTRIE

What to expect?

- **Introduction to Machine learning**
- **Clustering with DBSCAN**
    - Performance under pileup
- **Support Vector Machines (SVM)**
    - Hyperparameter Optimization
    - Case Studies
    - Implementation in the 8 TeV top squark search
- **Conclusion**

Machine learning

- Searching for new physics in HEP
  - Classification of Signal (New Physics) to the background (Standard Model).
  - For most of the new physics models idiom *looking for a needle in a haystack* does not actually suffice…

Machine learning

- A better version would be looking for a slightly different needle within a stack of needles.
- We need to analyze all the inputs in a very affective way.
  - Machine learning!
- Within HEP, the benefits are quite visible, the interest is high, but the support is limited.

Machine learning

- Machine learning: an autonomous process where the **P**erformance for a given **T**ask is improved by increasing **E**xperience. (T. M. Mitchell)
    - **T** — Classification of new physics events among standard model events, identification of particle of interest among vast noise…
    - **E** — Number of events: asymmetrical samples (ie most of the time input includes only 0.01% signal.)
    - **P** — "Discovery!" (or to be less dramatic sensitivity), correct identification, being resilient against pile-up…
- Rosetta for HEP - ML - Statistics (not true for all but safe to generalize)
    - *Label, Class*: *Signal* & *Background* (we would like to be more explicit… BTW *background* is *noise* for what it is worth and we use *noise* mainly for instrumental fluctuations)
    - *Performance: Sensitivity, significance*
    - *Performance criteria: Figure of Merit*
    - *Feature: Variable* (I know… It is harder to pronounce for non-native that is why it is preferred).

Machine learning

Data rate too high
@ 40 MHz

Low-level Trigger

Filtered data

Readout

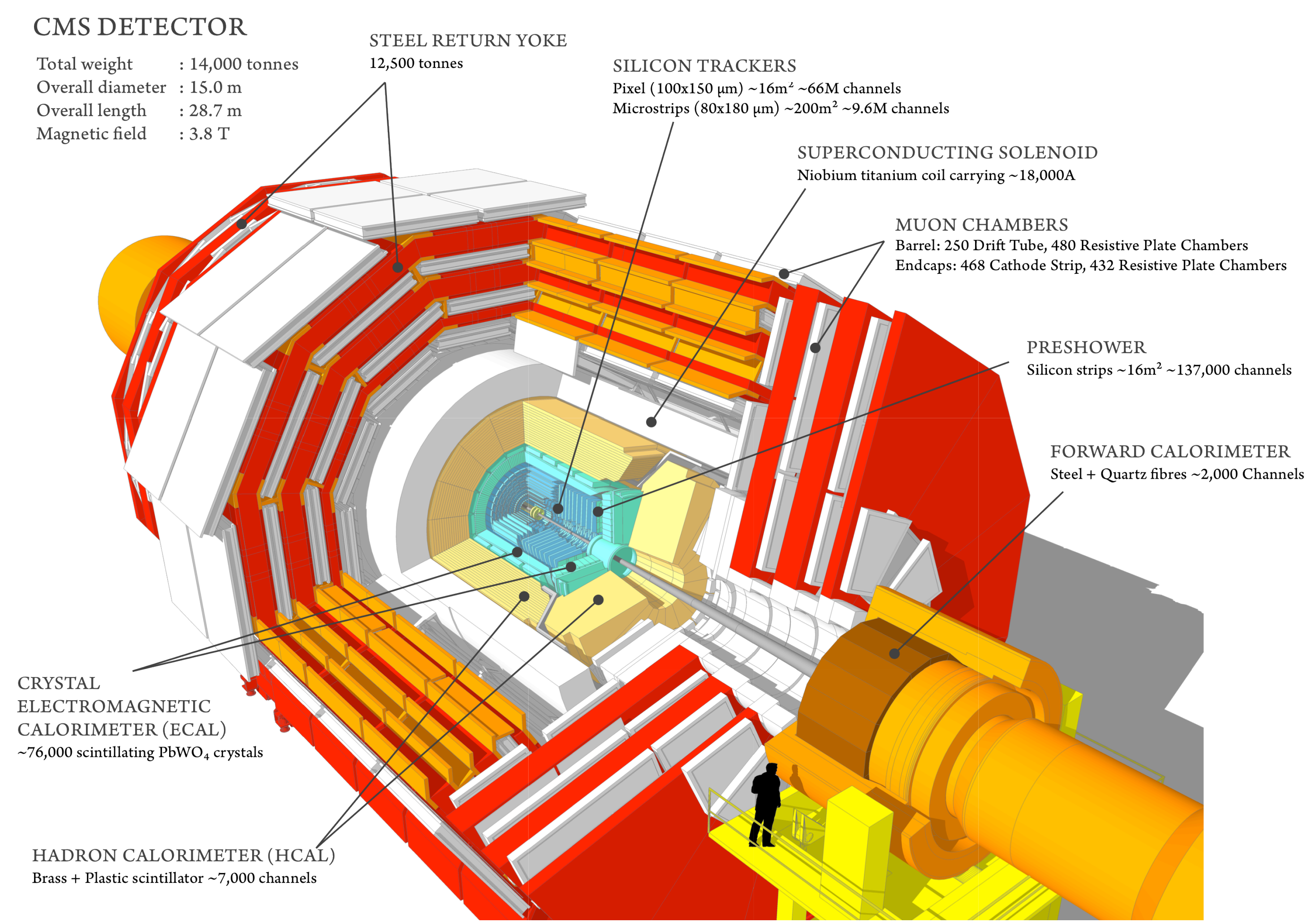
Data rate high
@ 100 KHz

High-level Trigger

Readout

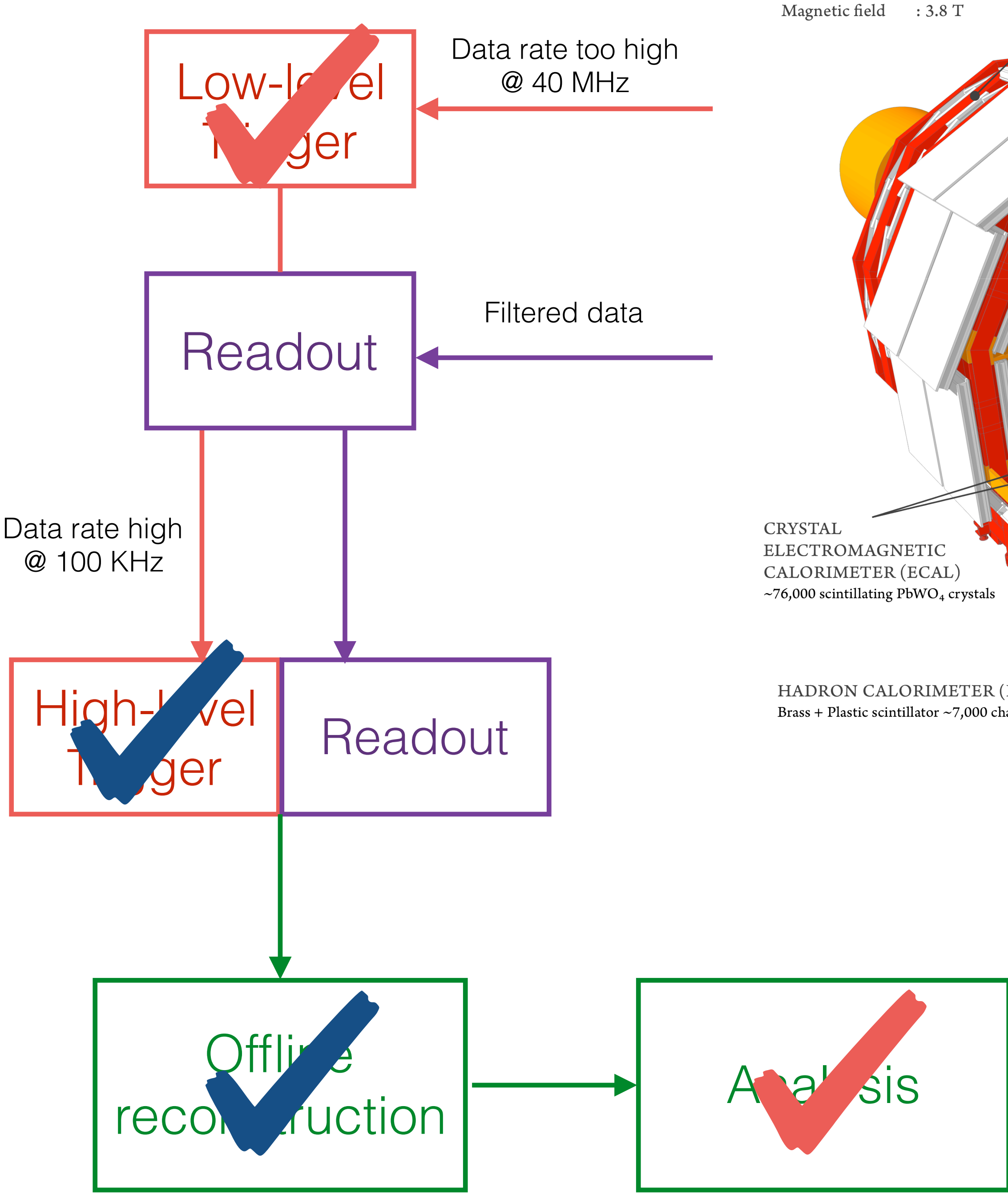
Offline reconstruction

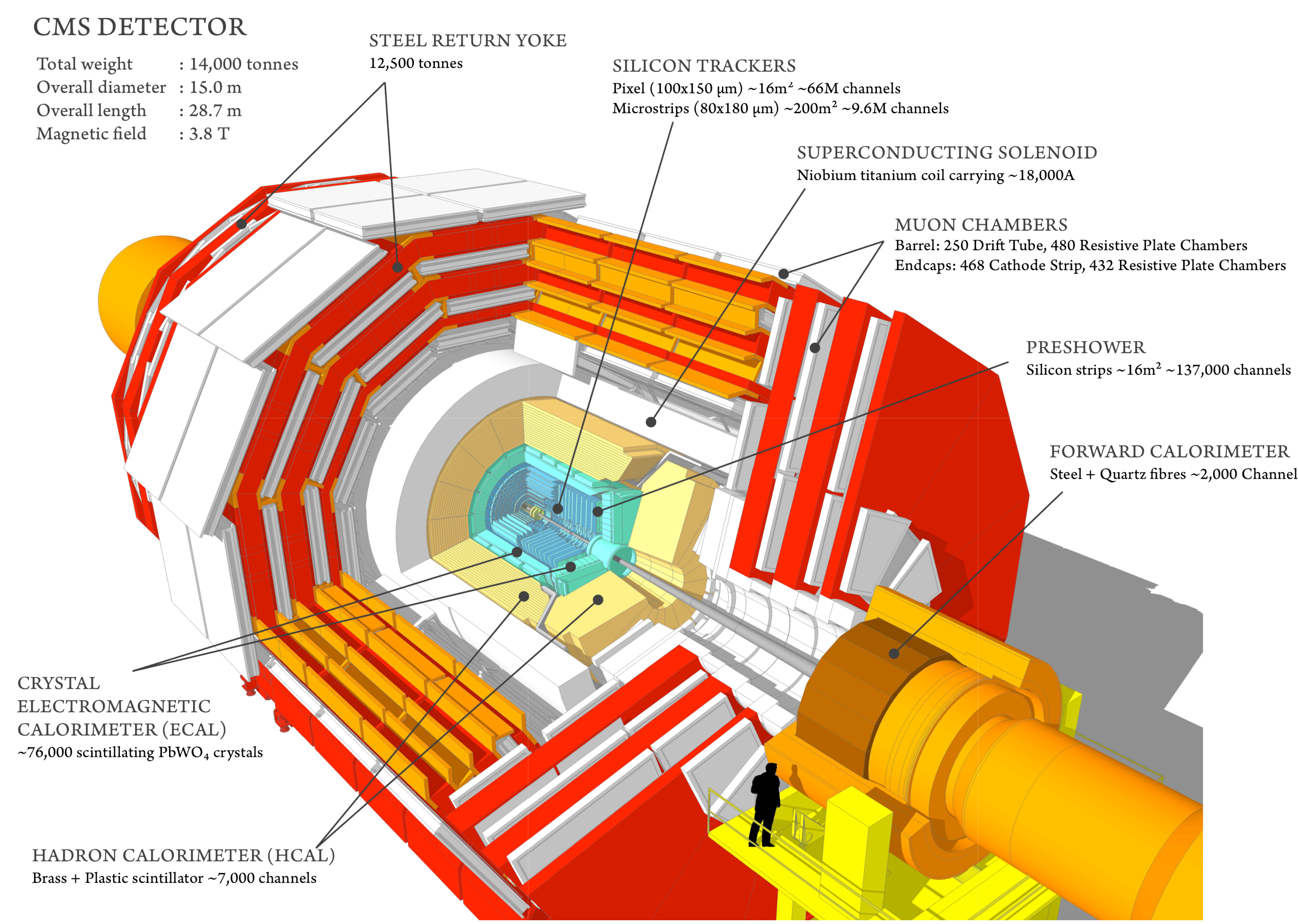
Analysis



An extremely simplified view of data path in CMS

Machine learning





An extremely simplified view of data path in CMS

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Machine learning

Supervised

- Decision trees
- Support Vector Machines
- Neural Nets
- Fischer discriminant
- ⋮

Unsupervised

- Hebbian learning
- Principal Component Analysis
- k-means
- DBSCAN
- ⋮

Machine learning

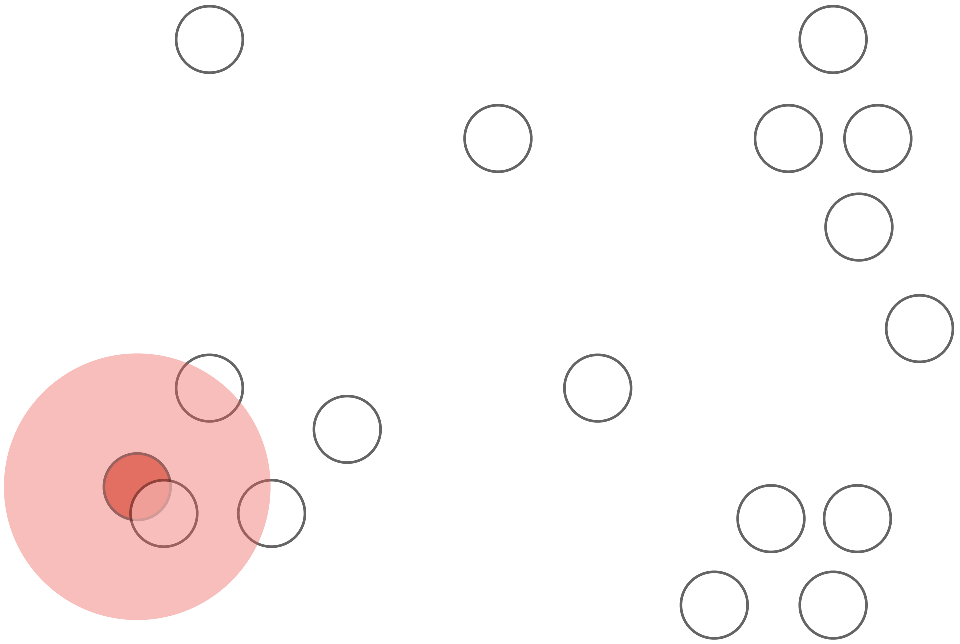
Supervised

- Decision trees
- Support Vector Machines
- Neural Nets (since 2013)
- Fischer discriminant
- ⋮

Unsupervised

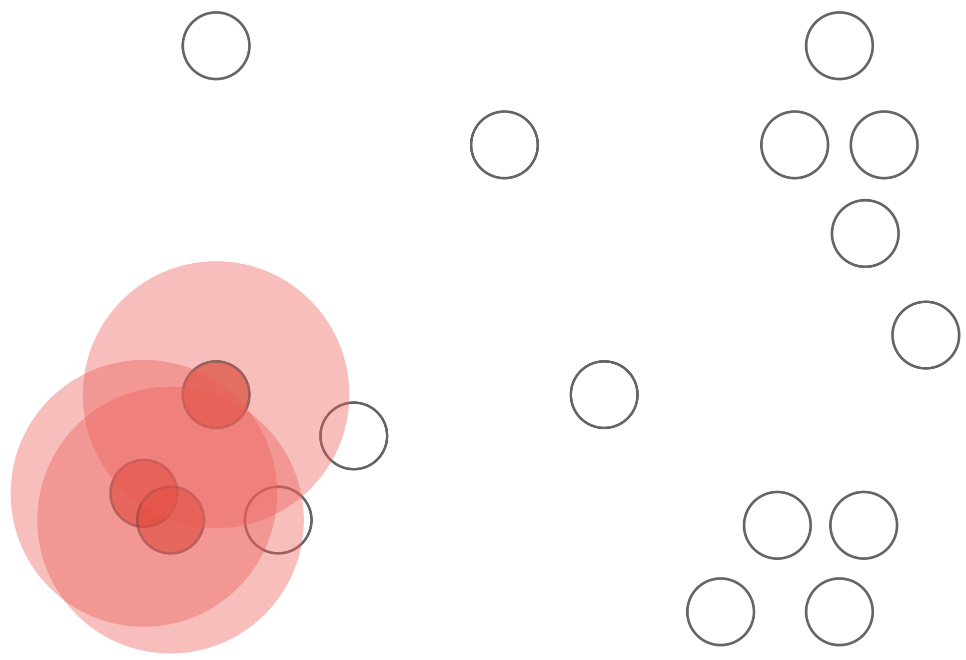
- Hebbian learning
- Principal Component Analysis
- k-means
- DBSCAN
- ⋮

DBSCAN



- DBSCAN is a an award winning (timing) density-based clustering algorithm. In this talk, this algorithm is compared to a simple cone algorithm.
- It has two hyperparameters: Minimum distance (radius) and minimum number of points.

DBSCAN



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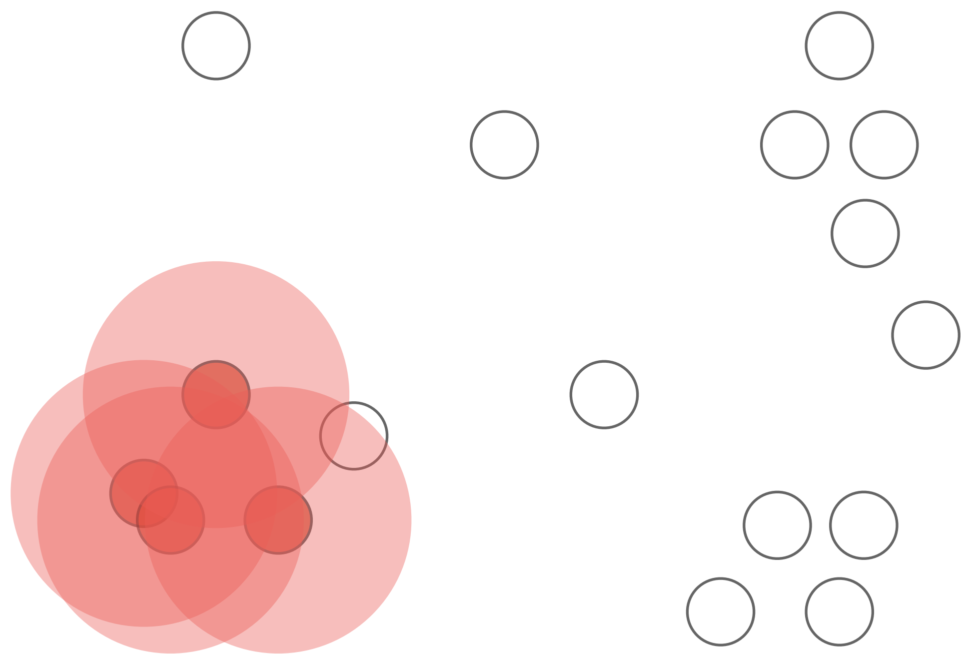
DBSCAN



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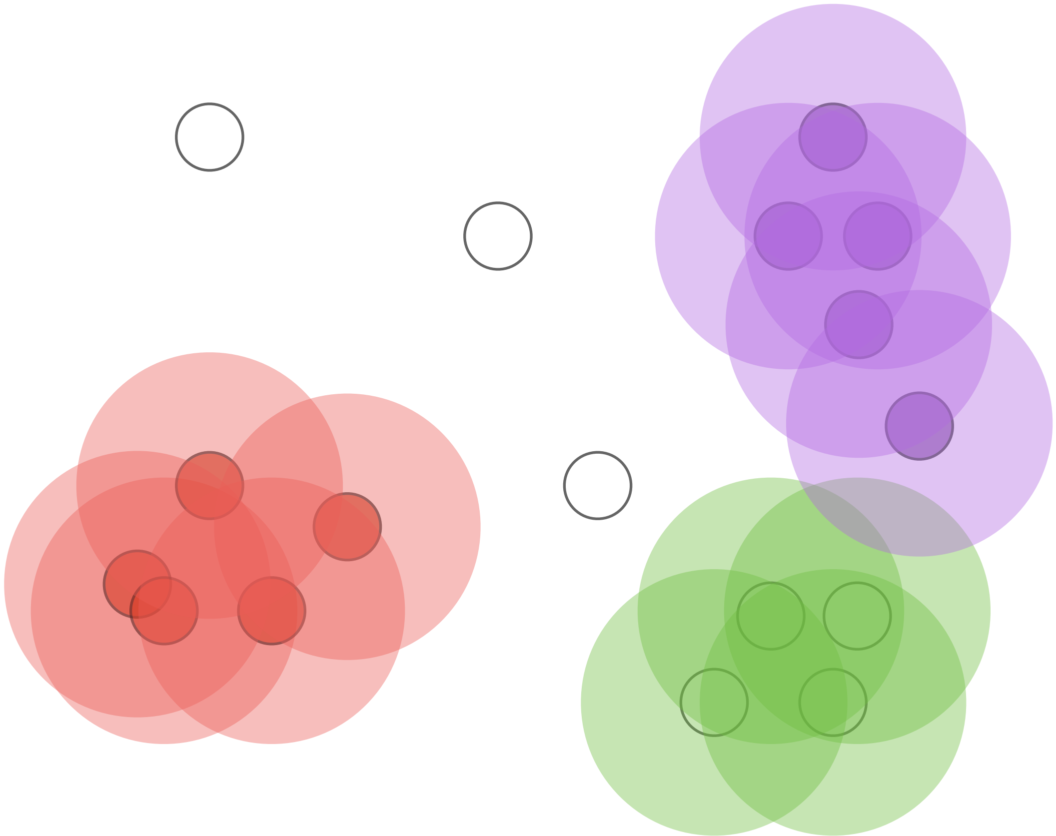
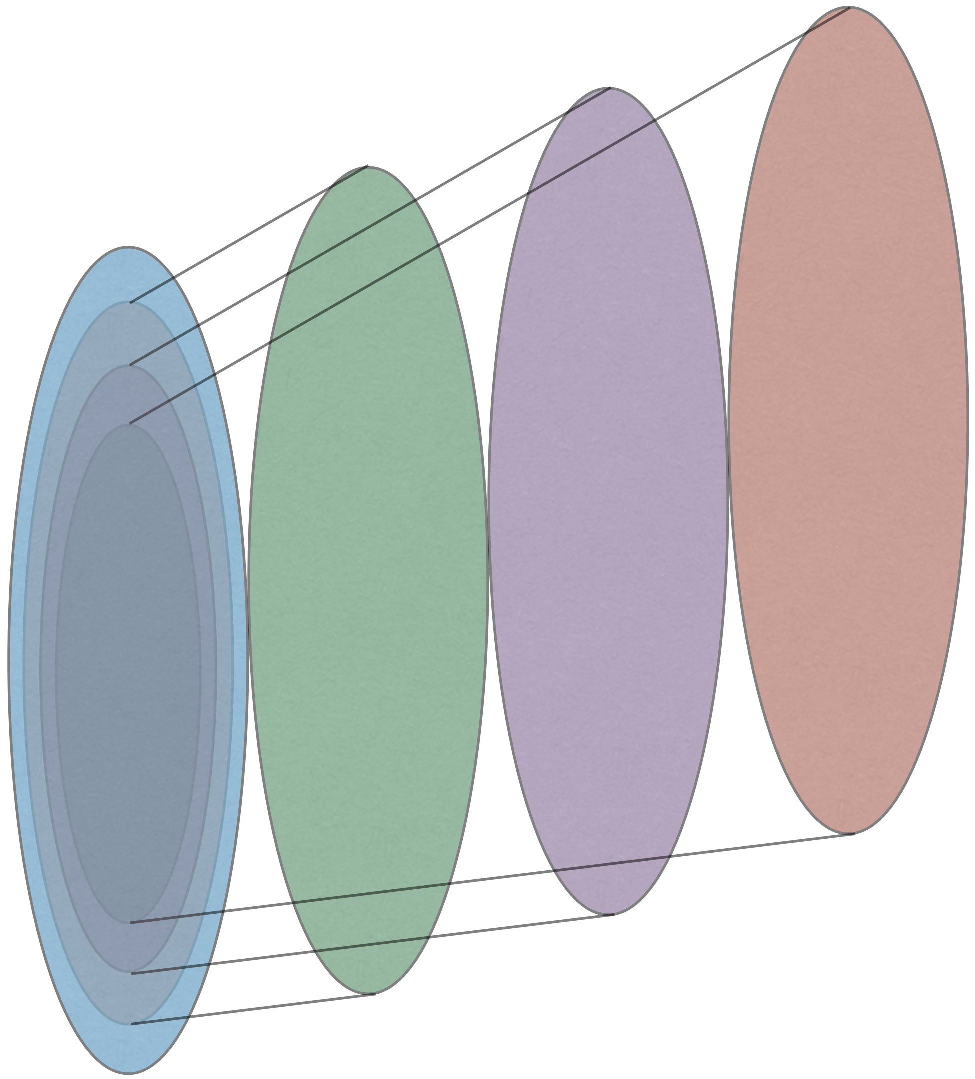
DBSCAN



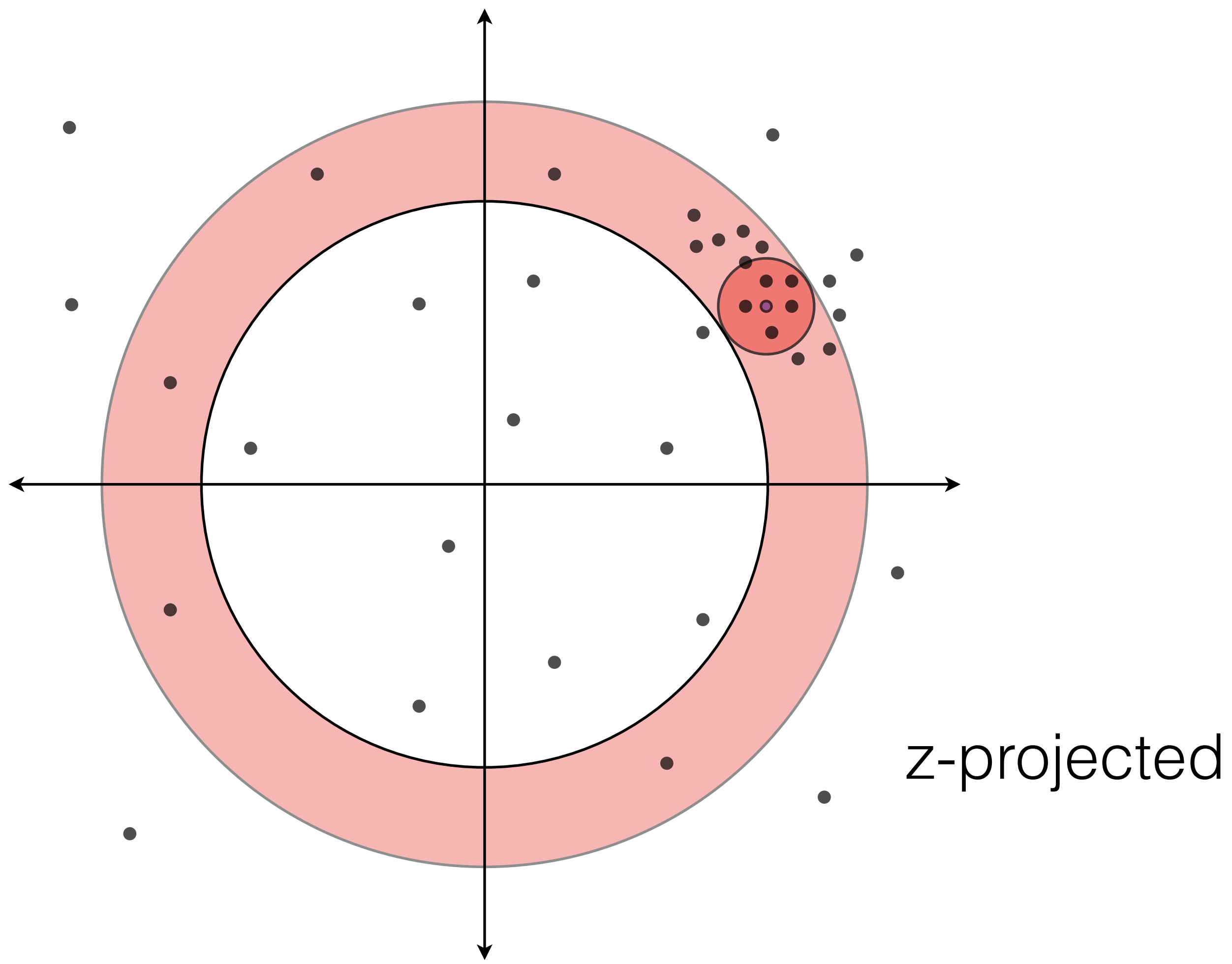
- DBSCAN is extremely efficient for
    - eliminating noise,
    - detecting non-uniform clusters.
- https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

Clustering algorithms



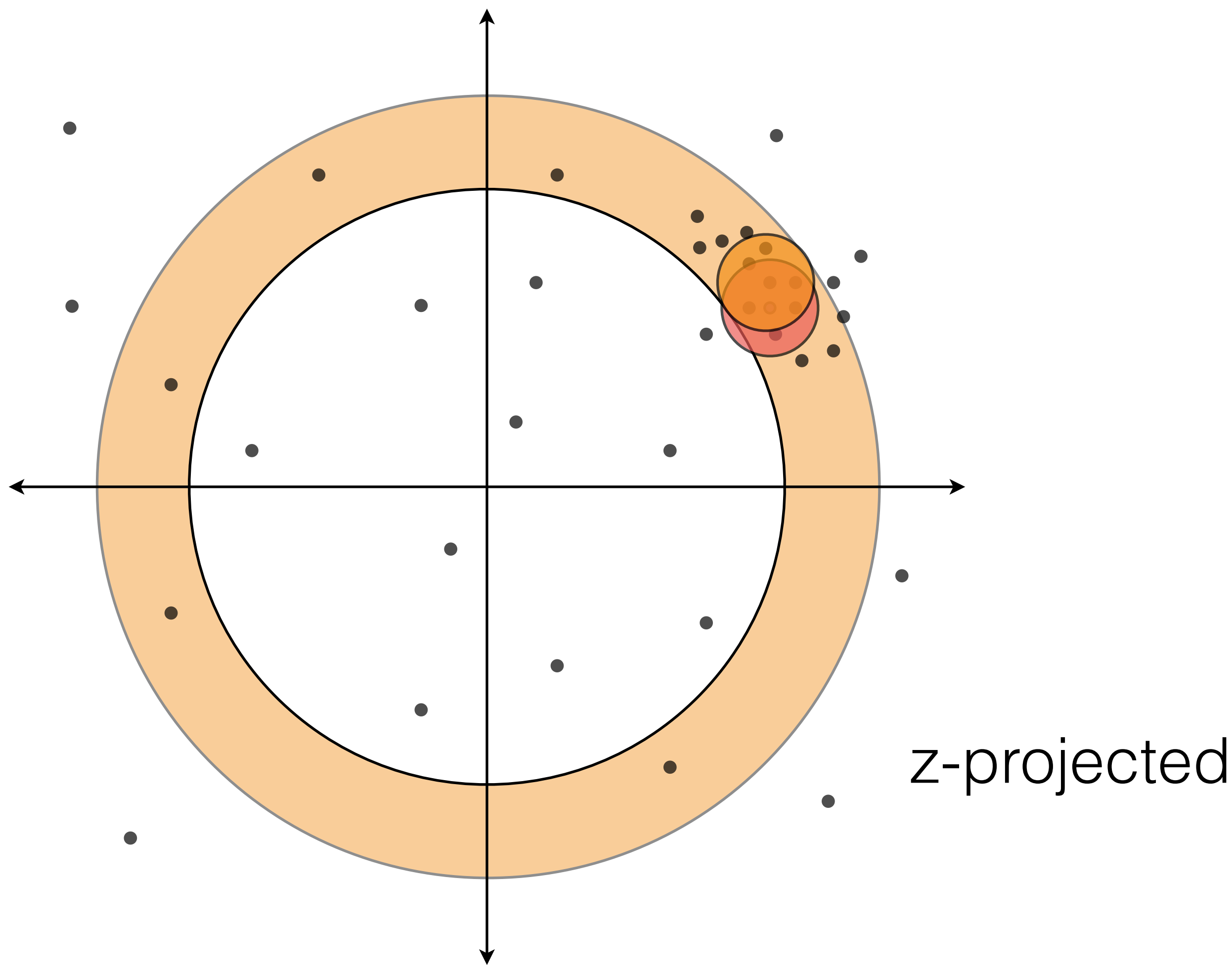
- To reconstruct the objects, we cluster the hits in our detectors using various algorithms. The readout is synchronous with LHC (ie ~40 MHz).
- These algorithms are meant to be implemented in low level electronics.
- In order to simplify the problem, a dimension reduction is performed by projecting the "layers" into a single plane in Z.

Software implementation



- The clusters are ranked wrt to distance to center.
- A secondary search is performed to find the neighbors.

Software implementation



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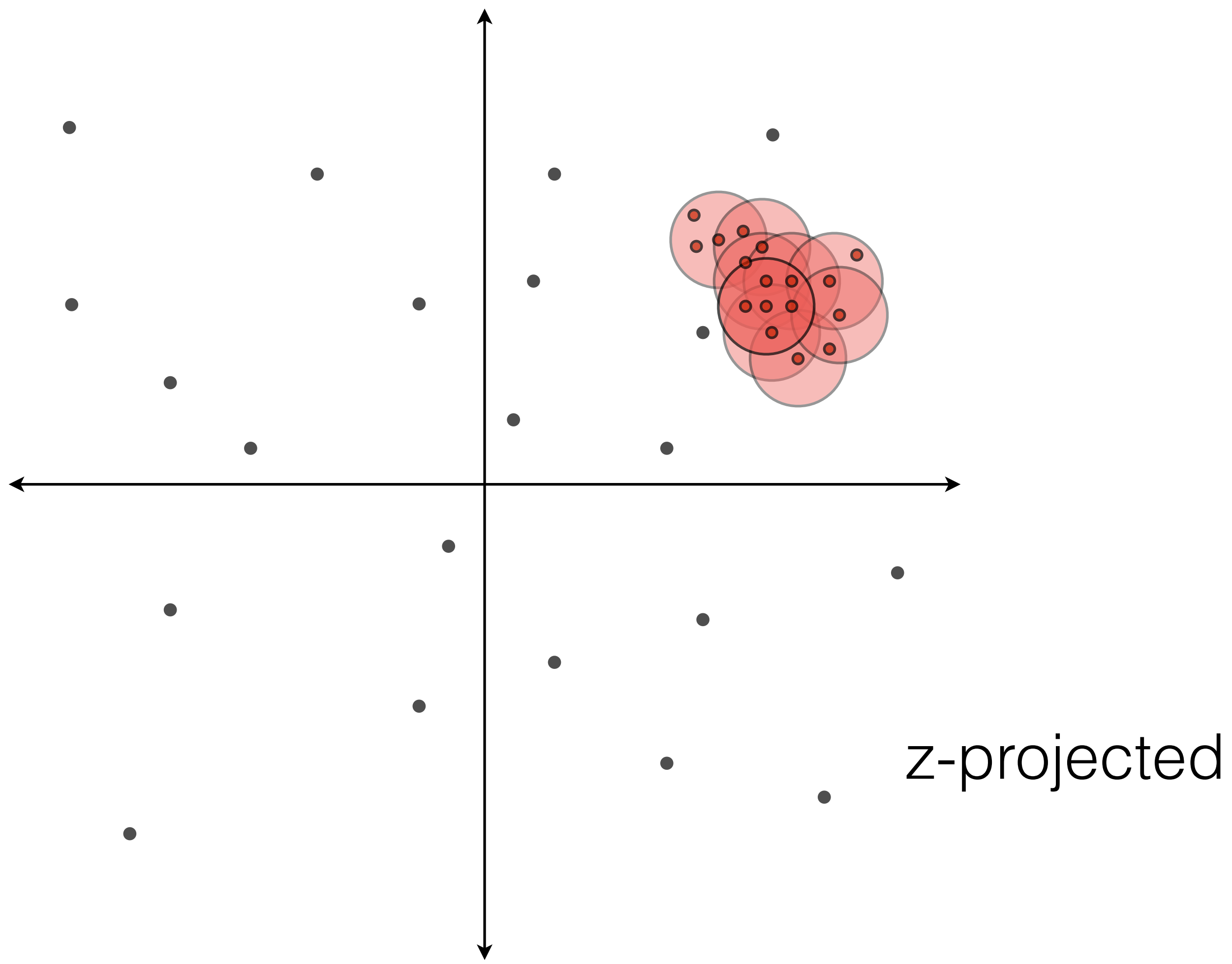
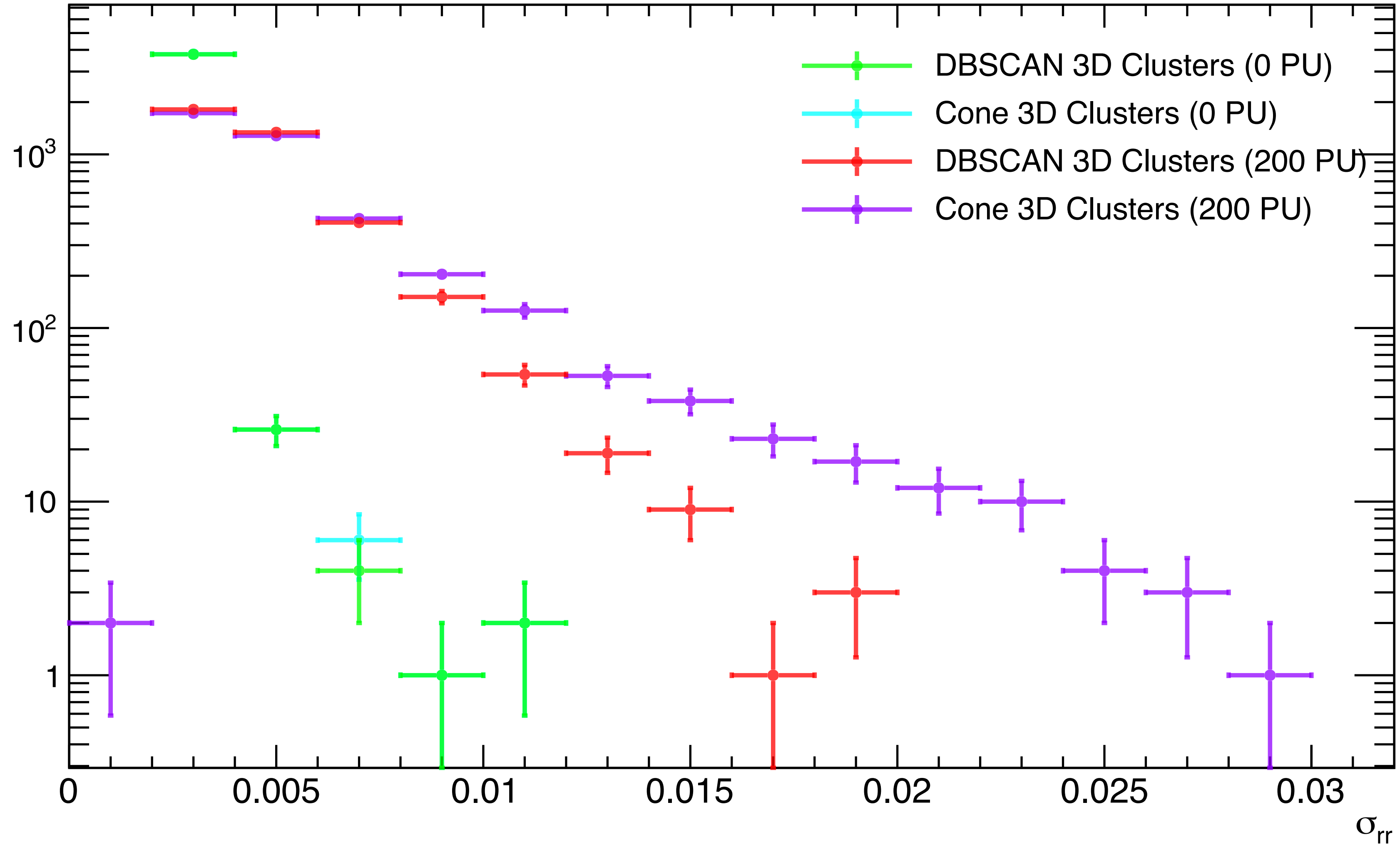
Software implementation



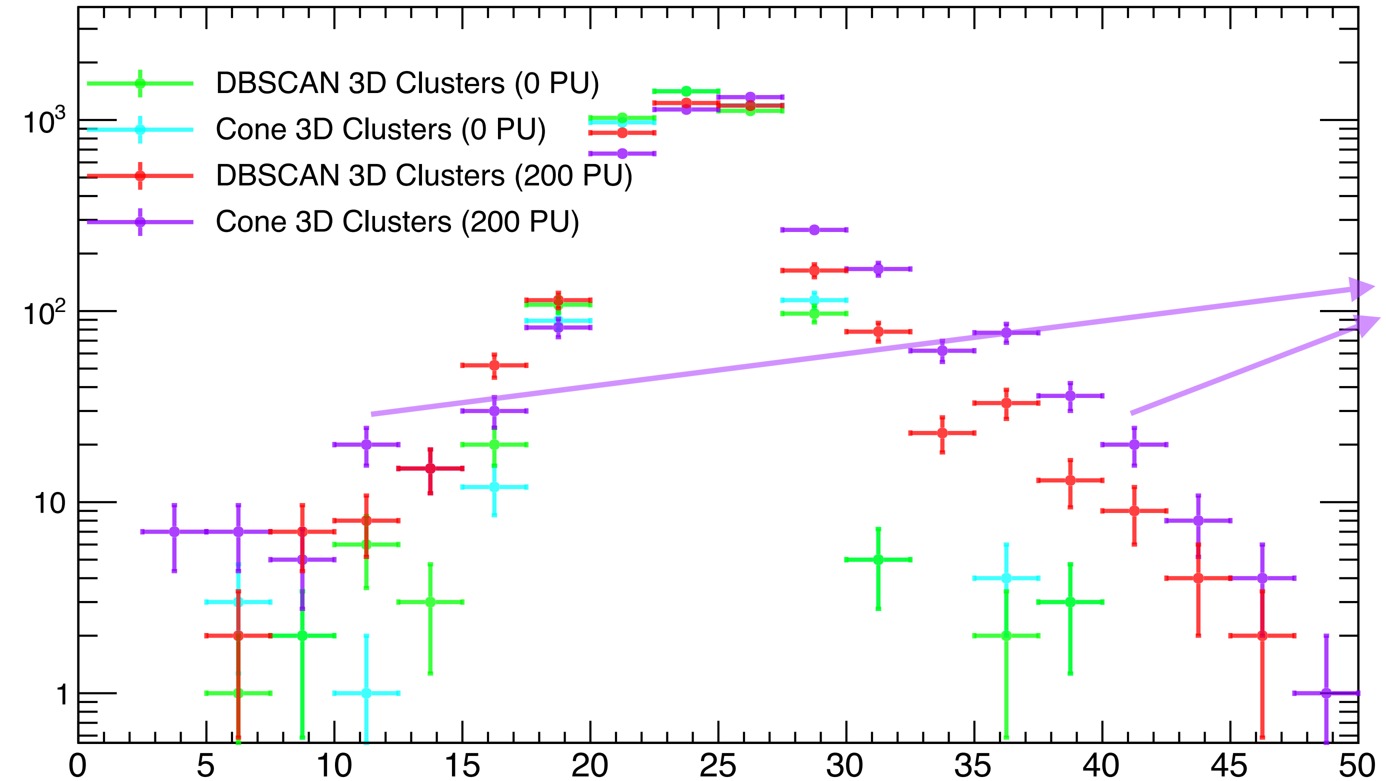
- The sorted DBSCAN algorithm is approximately 20 times faster than the unsorted search.
- The sorted DBSCAN is as fast as the Cone clustering algorithm.

Cluster shape comparison

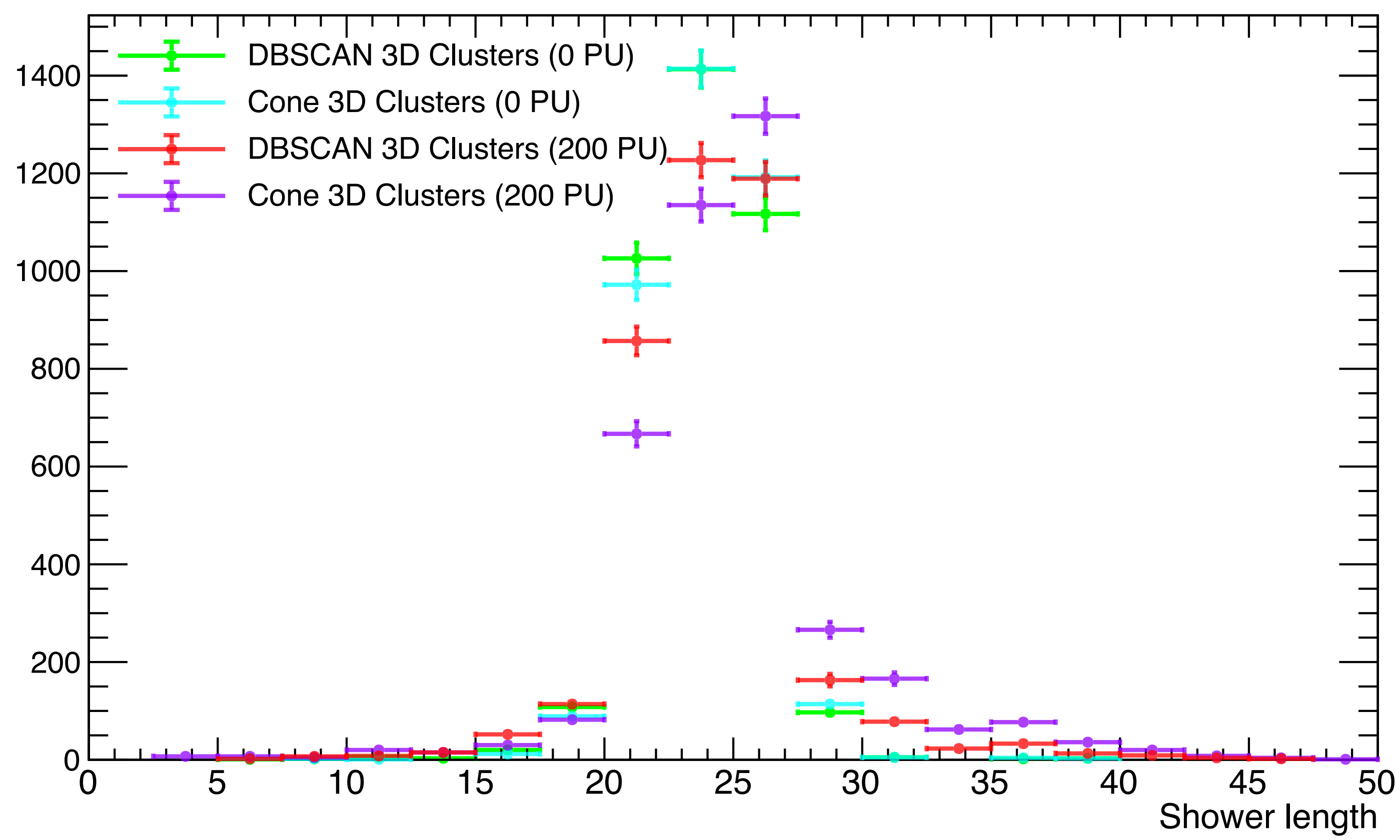


- With no PU, both algorithms produce clusters with similar widths (overlapping distributions).
- Even though it is still significantly affected by the high PU, the DBSCAN algorithm produces narrower clusters.

Cluster shape comparison



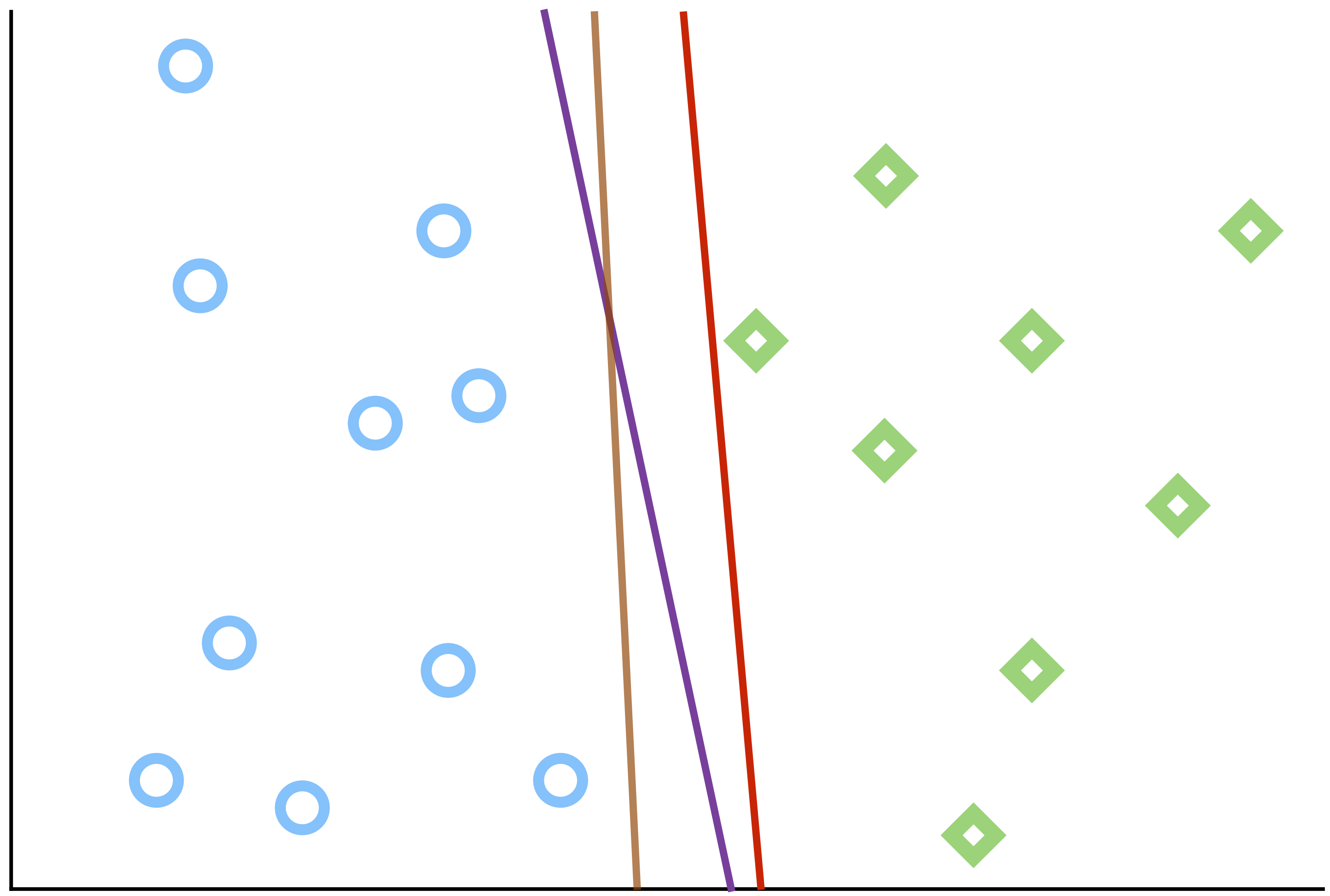
Cone algorithm yields to a wider shower length distribution in high PU



SVM

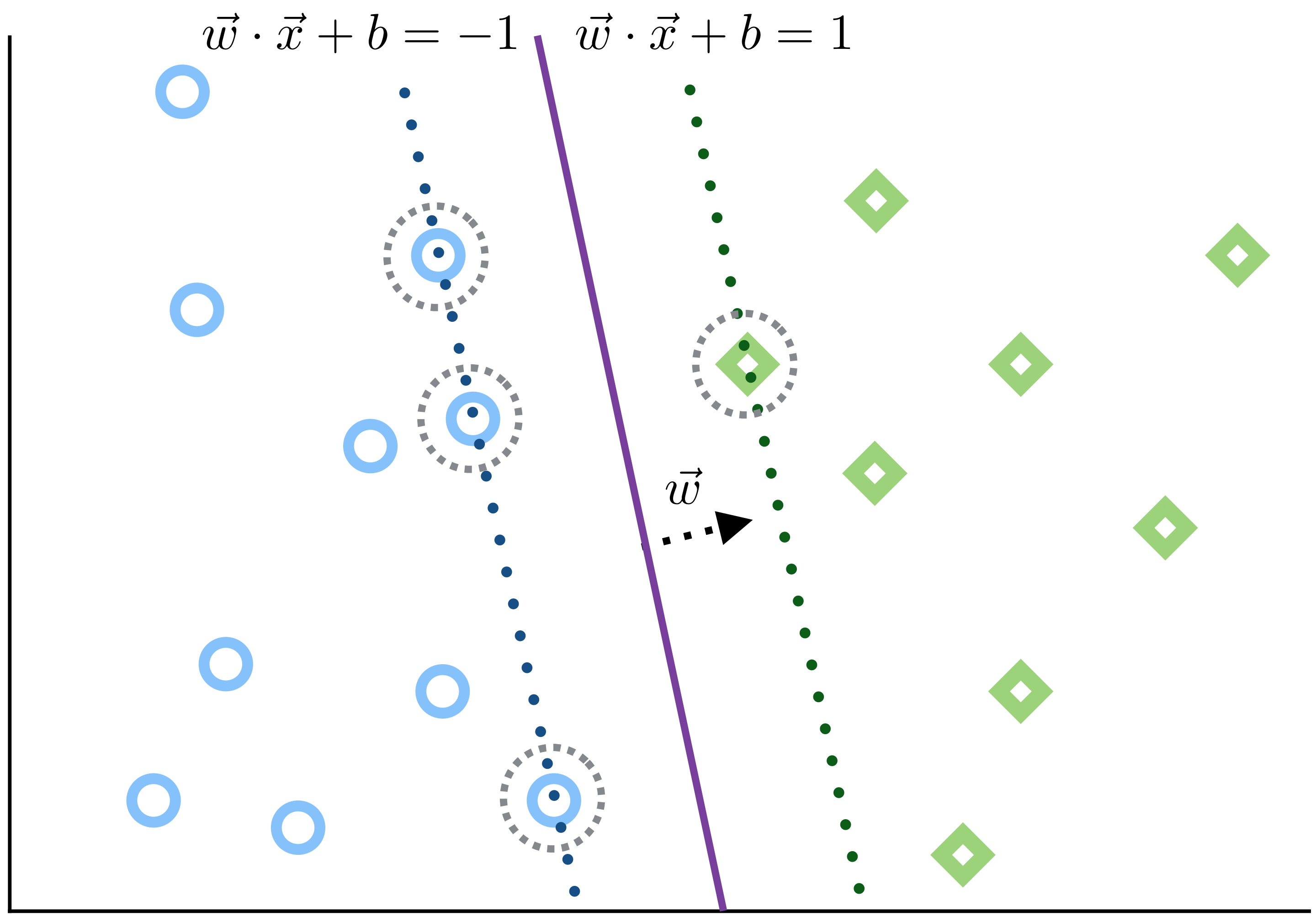
- As a rather modern machine learning algorithm, SVM is not widely used in the HEP data analysis, with few exceptions. In this talk I want to focus on this particular implementation.
- We used a discovery significance based hyperparameter tuning algorithm.
- We introduced an SVM classifier interface (SVM-HINT), which is based on a widely used SVM library (LIBSVM), tailored for HEP searches.
    - Performance and optimization of support vector machines in high-energy physics classification problems
    - https://github.com/ml-hint/svm-hint

Support Vector Machines



- What is the optimal way to separate two linearly separable distributions?

Support Vector Machines



- SVM provides a unique solution to separate two class problems i.e. signal from background.

$$\mathscr{L}(\vec{w}, \vec{x}, \alpha) = \frac{1}{2}|\vec{w}|^2 - \sum \alpha_i [y_i(\vec{w} \cdot \vec{x} + b) - 1]$$

Karush Kuhn Tucker Conditions

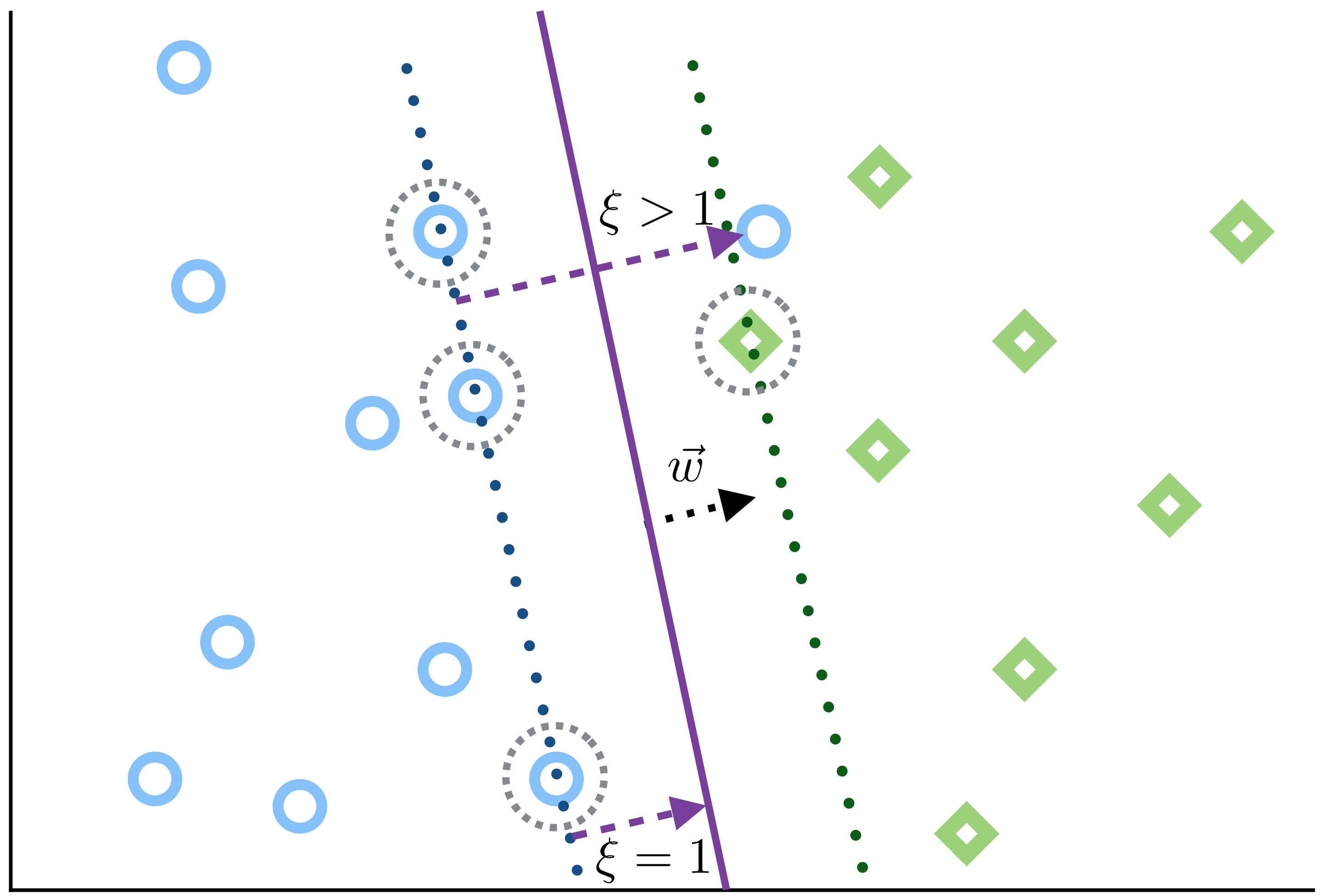
- If the problem has a solution and it satisfies the following conditions:

$$\vec{\alpha} \geqslant 0,$$
$$\alpha_i[y_i(\vec{w} \cdot \vec{x}_i + b) - 1] = 0, \qquad i = 1, ..., N.$$

- These conditions are known as the KKT conditions.

- The KKT conditions provide a generalization of the method of Lagrange multiplier for the case of inequalities .

Support Vector Machines

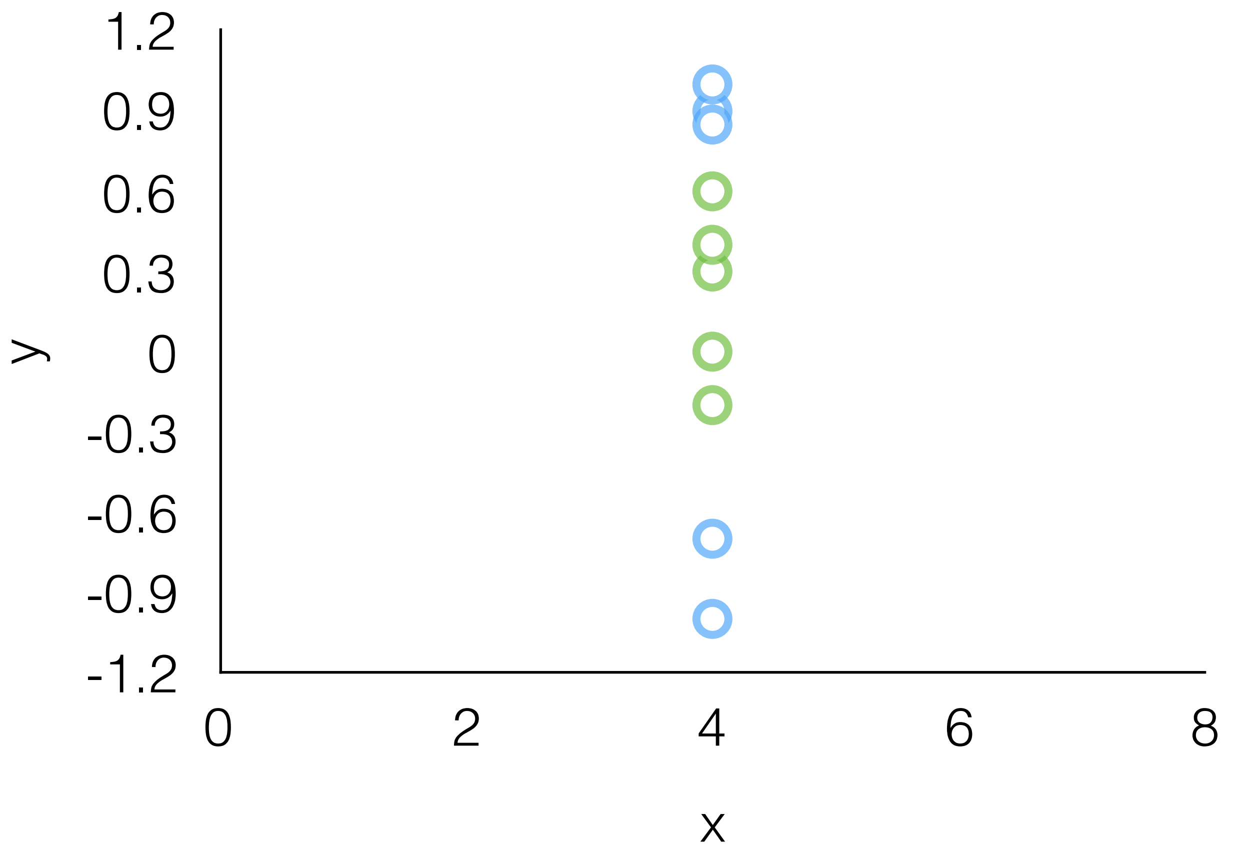


- Method of Lagrange multipliers — can be generalized respecting KKT conditions.
- Slack variables:

$$\mathscr{L} = \frac{1}{2}|\vec{w}|^2 + C\sum_i \xi_i - \sum \alpha_i[y_i(\vec{w}\cdot\vec{x}+b) - 1 + \xi_i] - \sum \beta_i \xi_i$$

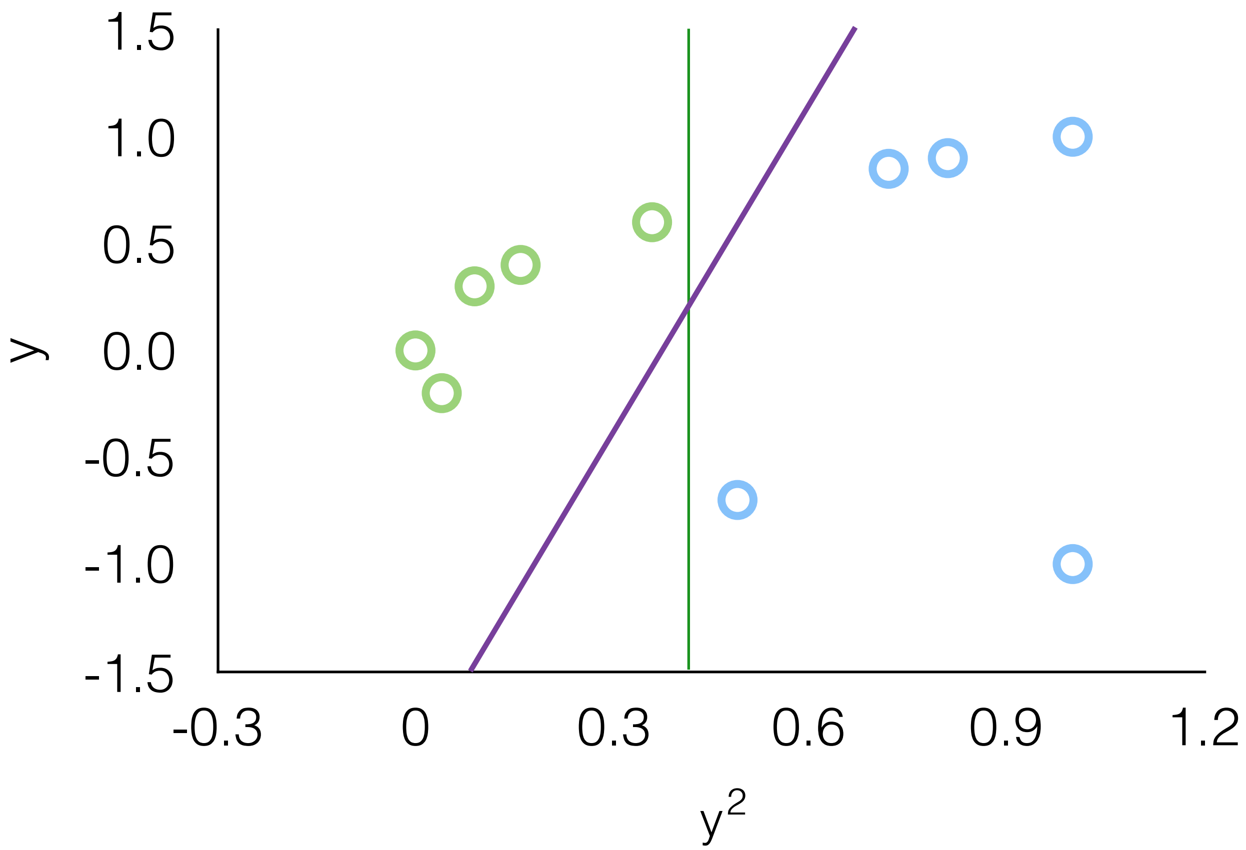
SVM: Non-linear case

- Is it possible to classify these samples with a linear decision function?



SVM: Non-linear case

- With a mapping in the form of $x \rightarrow y^2$
- Calculating a non-linear mapping may become cumbersome for large number of dimensions.



SVM: Non-linear case

- The decision function of SVM must be linear.
- Two non-linearly separable distributions can be linearly separable in a non-linearly transformed space.
- Calculating a non-linear mapping may become cumbersome for large number of dimensions (in some cases infinite).
- Way out: SVM uses a 'kernel trick' to circumvent this problem. By imposing the stability conditions, the Lagrangian can be reduced to the functional:

$$\mathscr{W}(\vec{\alpha}) = -\frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j (\vec{x}_i \cdot \vec{x}_j) + \sum \alpha_i$$

- Various kernels are available (Mercer's theorem). In this study, RBF (Radial Basis Function) kernel is used:

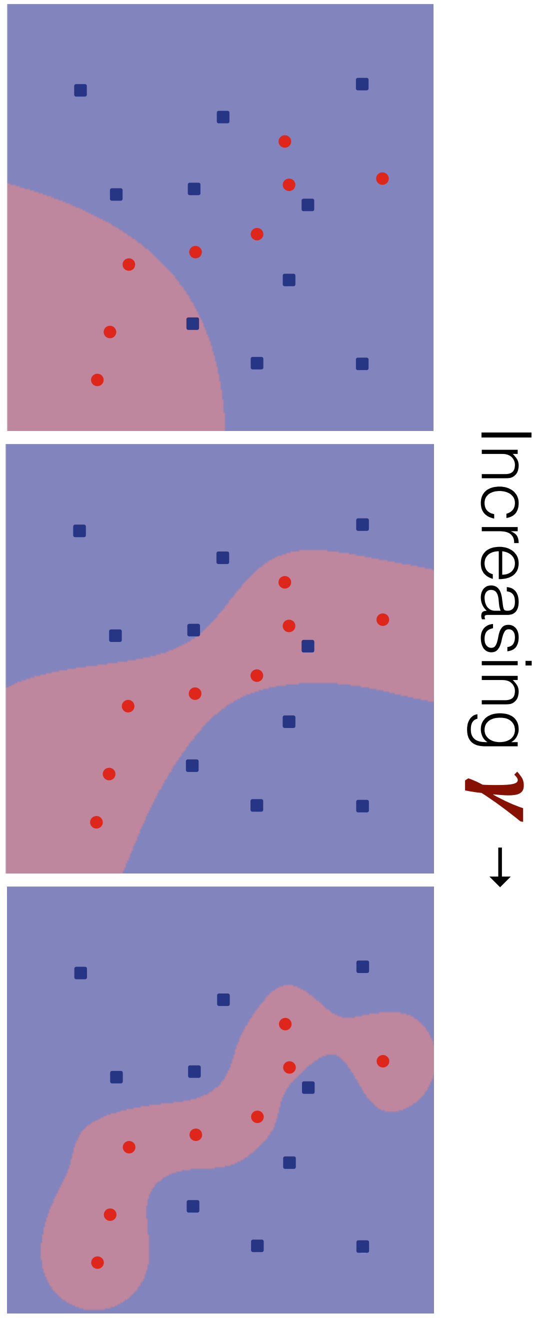
$$K(\vec{x}_i, \vec{x}_j) = e^{-\gamma|\vec{x}_i - \vec{x}_j|^2}$$

libSVM

- libSVM (Chang et. al.) is a well tested and widely used SVM library.
  - http://www.csie.ntu.edu.tw/~cjlin/libsvm/
- libSVM is using an improved version of Sequential Minimal Optimization.
- The library is optimized and tested over many years.

Hyperparameter optimization

- SVM with RBF kernel has two hyper-parameters which need to be set before the application:
  - the slack variable parameter **C**,
  - the inverse kernel width $\boldsymbol{\gamma}$.
- A discovery significance based algorithm outperforms other performance measures for the physics searches.
- We implemented a custom grid search algorithm for the Hyper-parameter optimization based on the Asimov significance estimator.



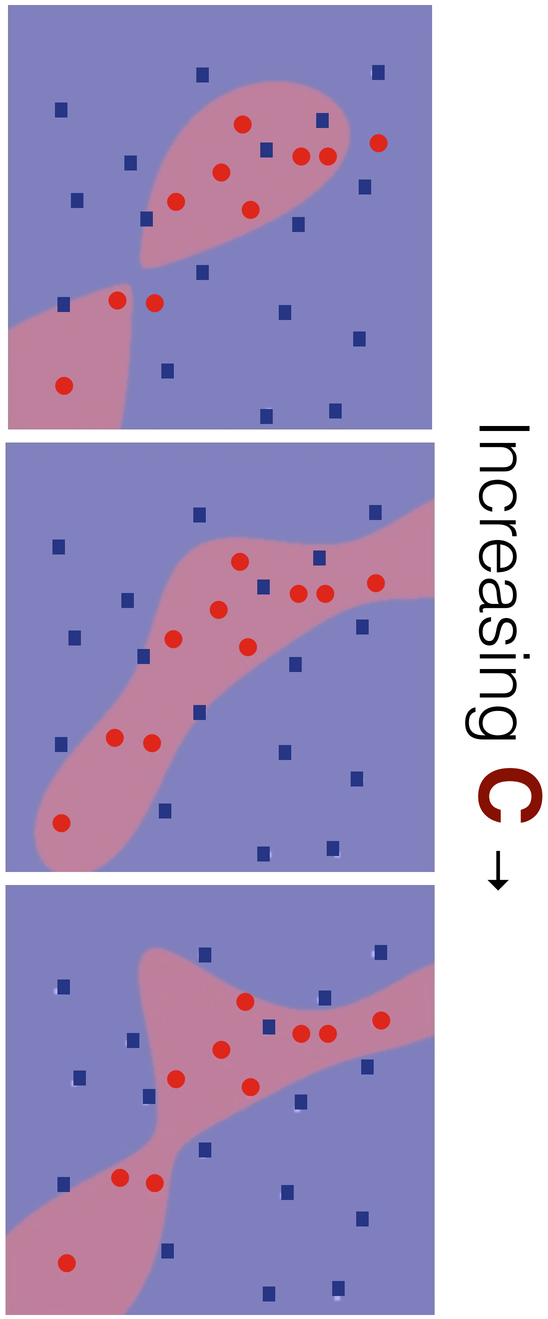
Two classes: Blue is background and red is signal

Hyperparameter optimization

- A custom iterative grid search algorithm is employed to optimize the hyper-parameters:
  - In order to prevent over-training in the least computationally cumbersome way:

    $$\tilde{Z} = Z_A^{(\text{test})}\left[1 - \frac{|Z_A^{(\text{test})} - Z_A^{(\text{train})}|}{Z_A^{(\text{test})} + Z_A^{(\text{train})}}\right]$$

  - Starting from an initial set, **C** and $\boldsymbol{\gamma}$ parameters are scanned with a focusing parameter (see the next slide)



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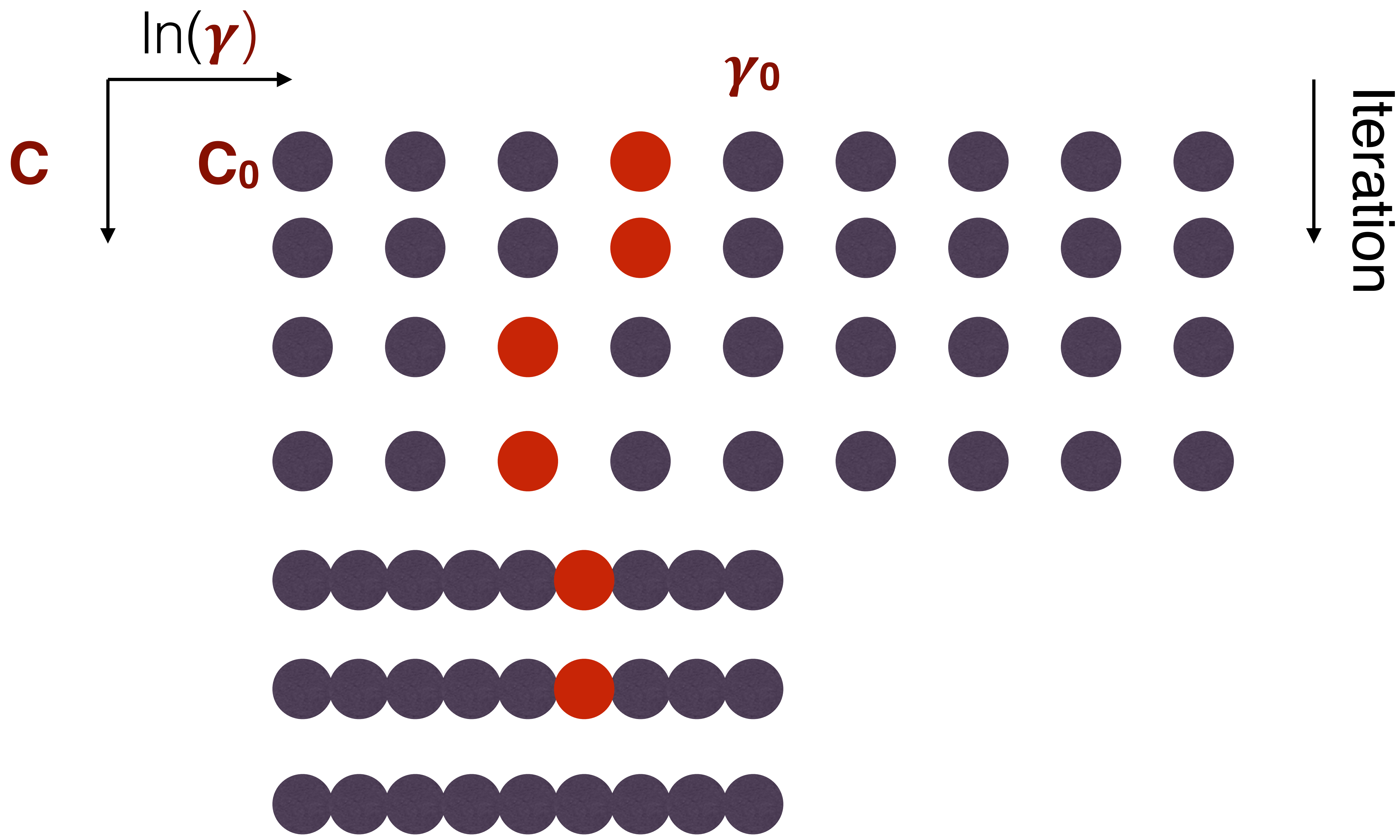
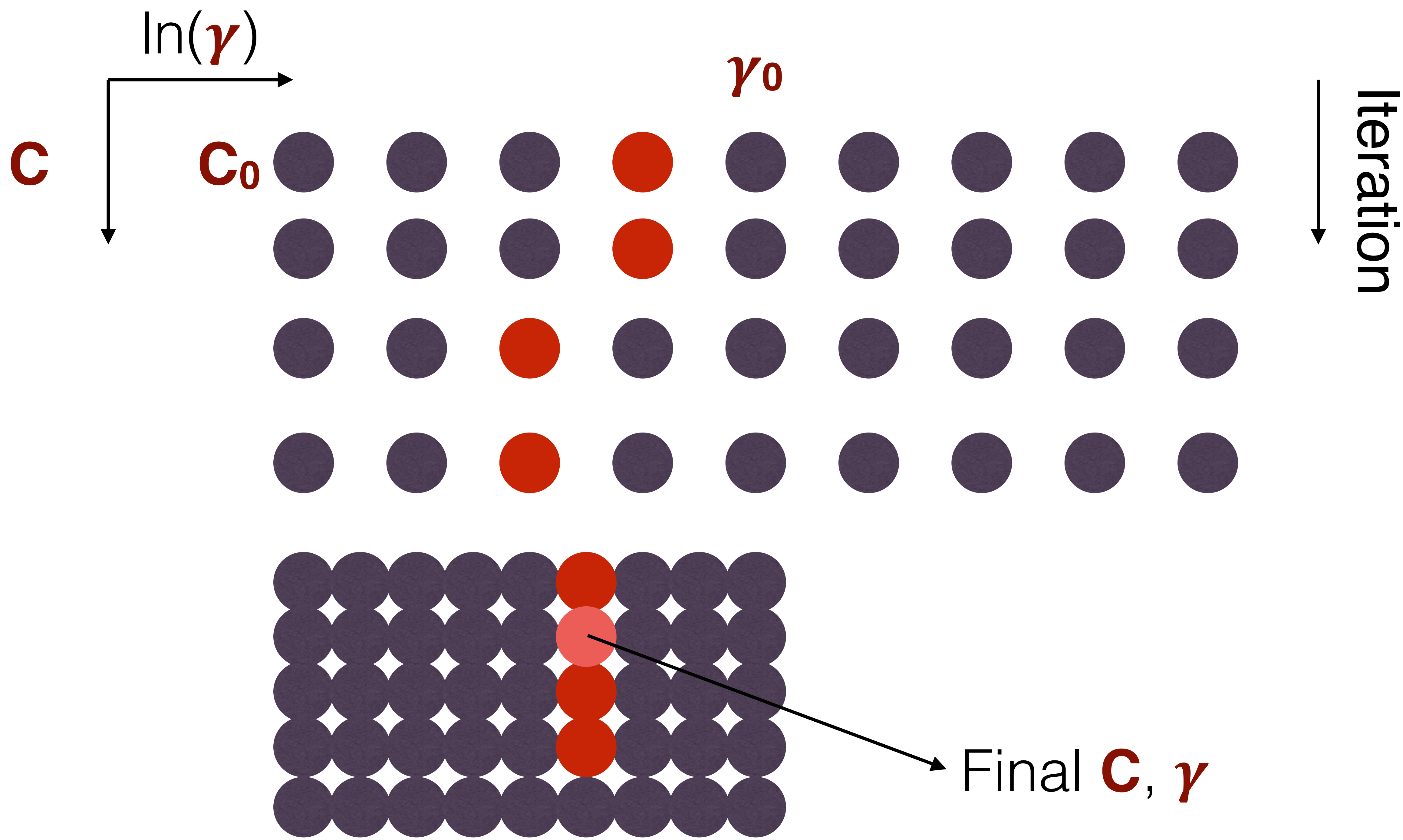
Hyperparameter optimization



Hyperparameter optimization



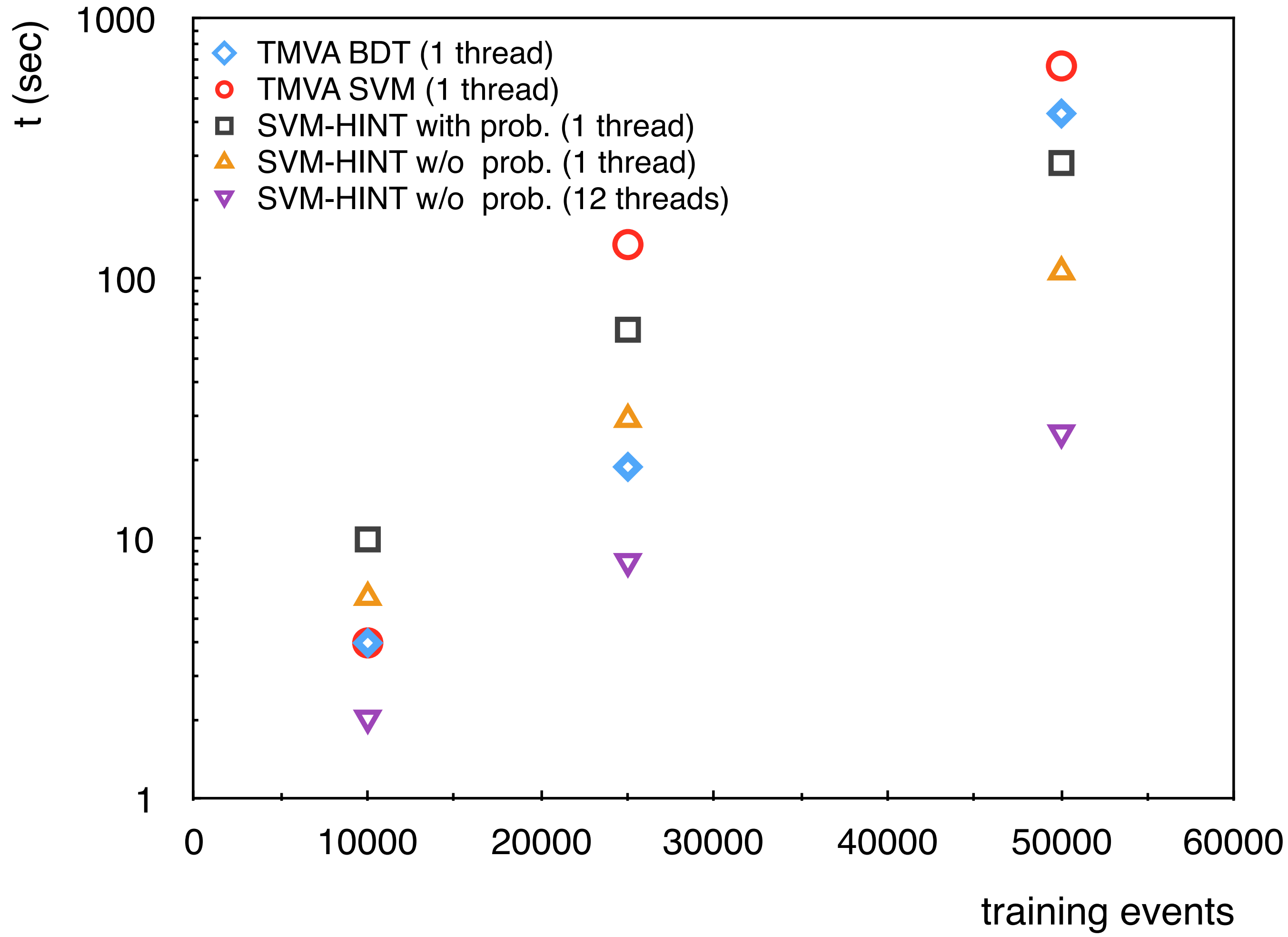
Case Study I

- A simple toy example is used to compare the time performance of the implementations.
- The variables are sampled from:

$$\begin{array}{lcll} V_1 = & \sin(x_1); & & x_1 \sim g(x_1|a,b) \\ V_2 = & x_2; & & x_2 \sim \exp(-x_2/c) \\ V_3 = & x_3; & & x_3 \sim g(x_3|d,e) \\ V_4 = & \sqrt{x_4}; & & x_4 \sim \exp(-x_4/f) \end{array}$$

- TMVA-BDT is used as a benchmark implementation.

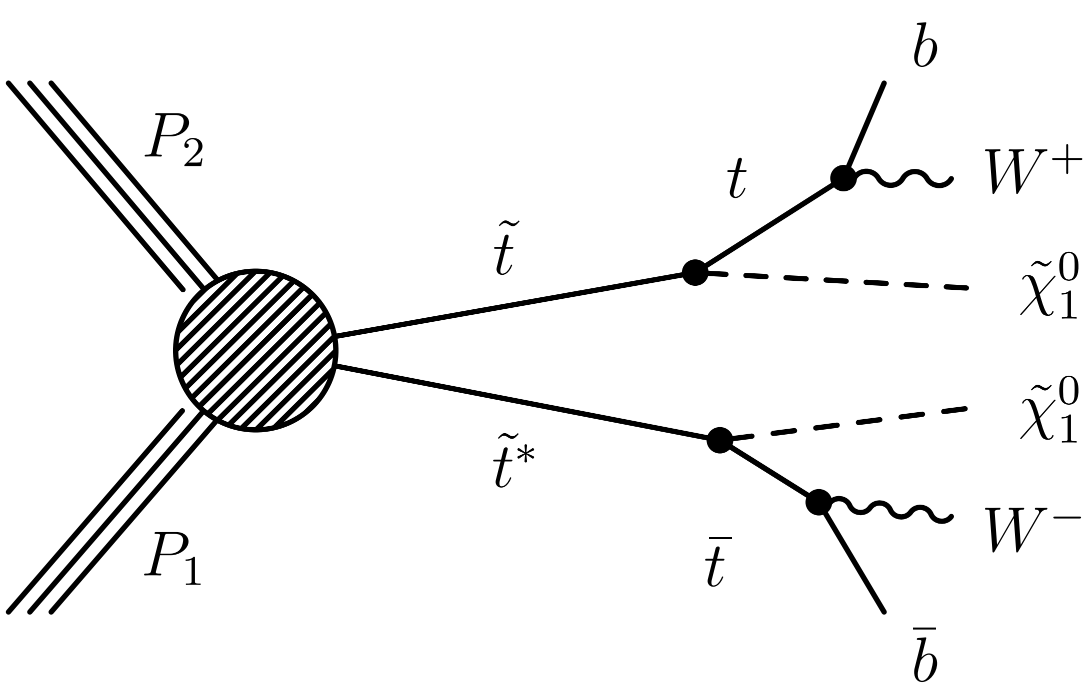
Case Study I: Runtime performance



- The algorithms are optimized to have similar accuracies.
- SVM-Hint with 12 threads has the **fastest timing performance**.
- SVM-Hint scales with number of training events.
- BDT almost competitive in speed with lower number of training events.

Case Study II

- Search for supersymmetry in single lepton final states (14 TeV).
- A benchmark SUSY model - an SMS simplified model. The particular mass parameters: Top quark super partner mass of 900 and LSP mass 100 GeV.
- Only the dominant SM background $t\bar{t} \to l(l + \mathrm{jets})$ is and only this background is considered for the sake of simplicity.
- Simulations performed with Delphes fast simulation program including pileup (same as used for Snowmass study)



T2tt

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Case Study II

- 25 variables are considered to discriminate signal and background.
- The variables are grouped into four different sets with respect to their complexity.
- Low-level variables include basic features of physics objects whereas high-level variables are constructed from these objects.
- TMVA-BDT is used as a benchmark implementation.

	Variable	Set 1	Set 2	Set 3	Set 4
low-level	$p_{\mathrm{T},l}$	•	•		
	η_l	•	•		
	$p_{\mathrm{T},jet(1,2,3,4)}$	•	•		
	$\eta_{jet(1,2,3,4)}$	•	•		
	$p_{\mathrm{T},b\,jet1}$	•	•		
	$\eta_{b\,jet1}$	•	•		
	n_{jet}	•	•		
	$n_{b\,jet}$	•	•		
	$\not{E}_{\mathrm{T}}$	•	•		•
	H_{T}	•	•		•
high-level	m_{T}	•		•	•
	m_{T2}^{W}	•		•	•
	$\Delta\phi(W,l)$	•		•	
	$m(l,b)$	•		•	
	Centrality	•		•	
	Y	•		•	
	H_{T}-ratio	•		•	
	$\Delta\mathrm{r}_{\min}(l,b)$	•		•	
	$\Delta\phi_{\min}(j_{1,2},\not{E}_{\mathrm{T}})$	•		•	

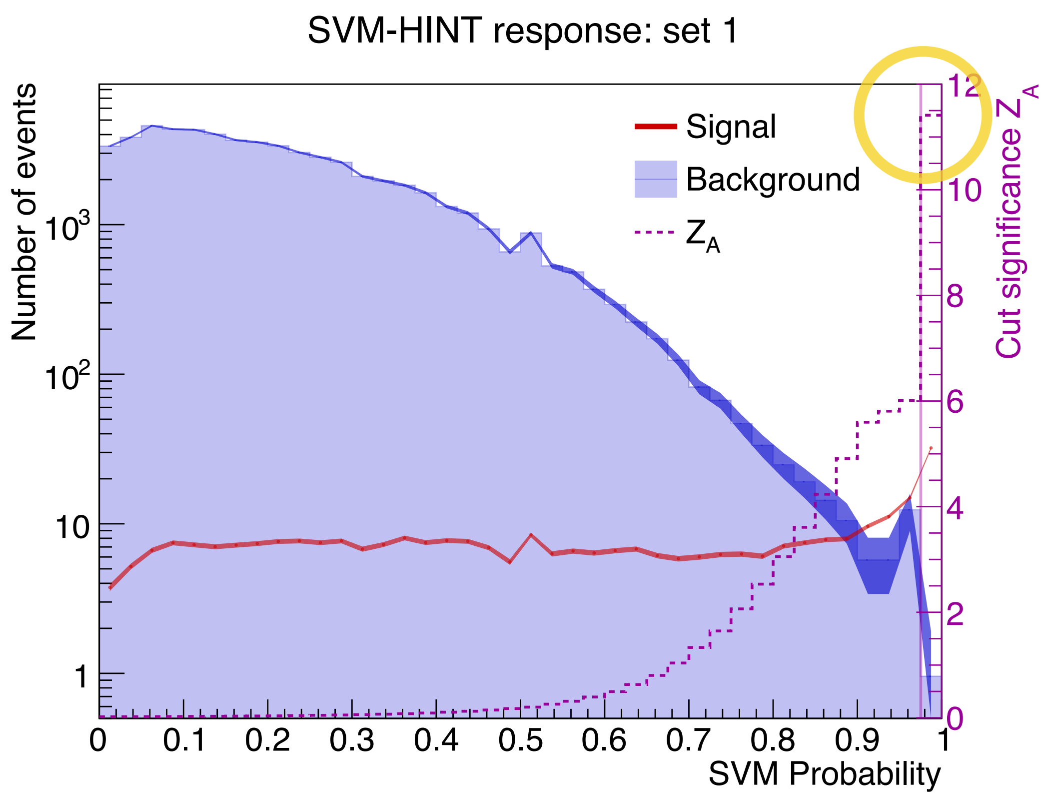
SVM-HINT

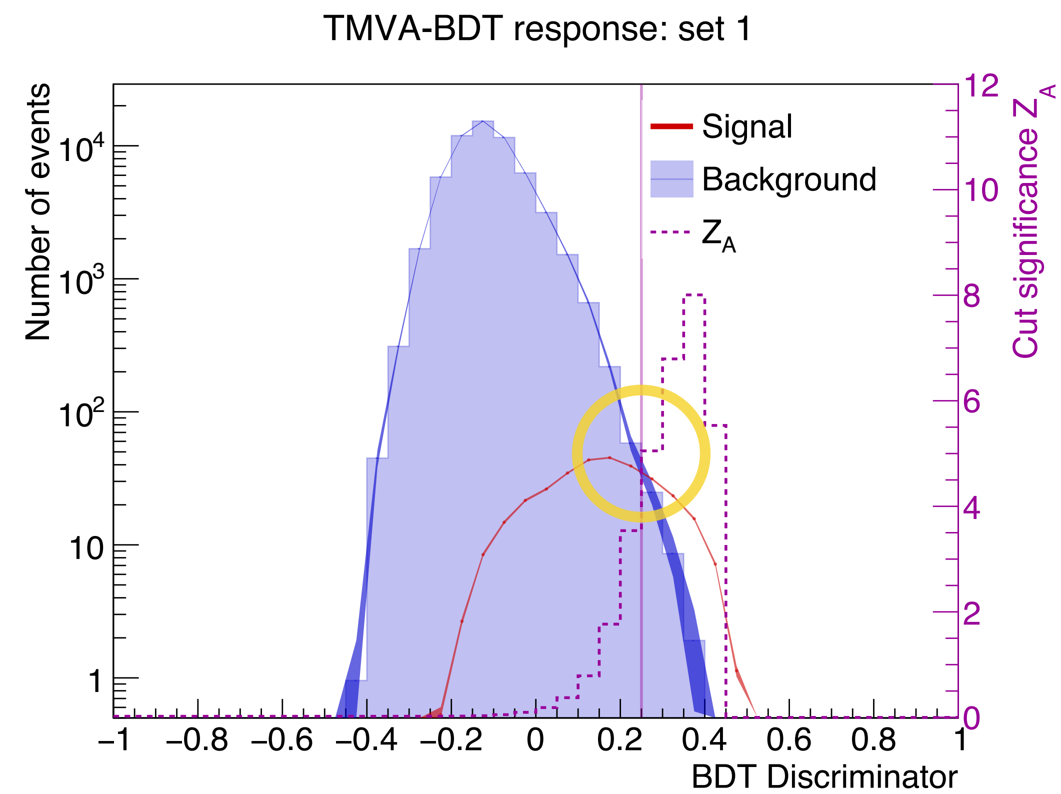
	SVM-HINT			TMVA-BDT			
Set	N_s	N_b	$Z_A^{\max}$	N_s	N_b	$Z_A^{\max}$	Z_A^{prov}
1	32.1 ± 0.6	1.0 ± 1.0	11.4	24.1 ± 0.5	1.9 ± 1.4	8.0	5.1
2	23.2 ± 0.5	23.9 ± 4.8	2.5	16.2 ± 0.4	10.5 ± 3.2	3.0	1.5
3	37.8 ± 0.6	9.6 ± 3.0	6.1	40.5 ± 0.7	9.6 ± 3.0	6.4	3.7
4	33.4 ± 0.6	20.1 ± 4.4	3.7	40.5 ± 0.7	35.4 ± 5.8	3.0	1.8

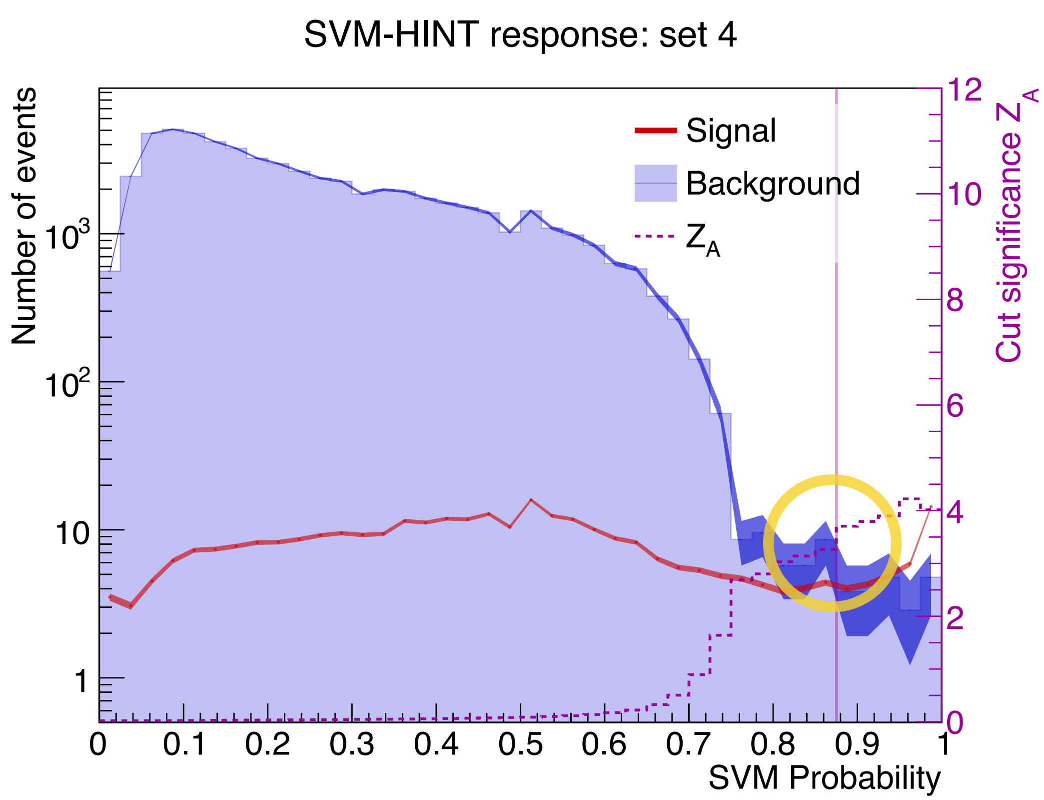
- https://github.com/ml-hint/svm-hint
- SVM-HINT provides typically **strong classification out of the box.**

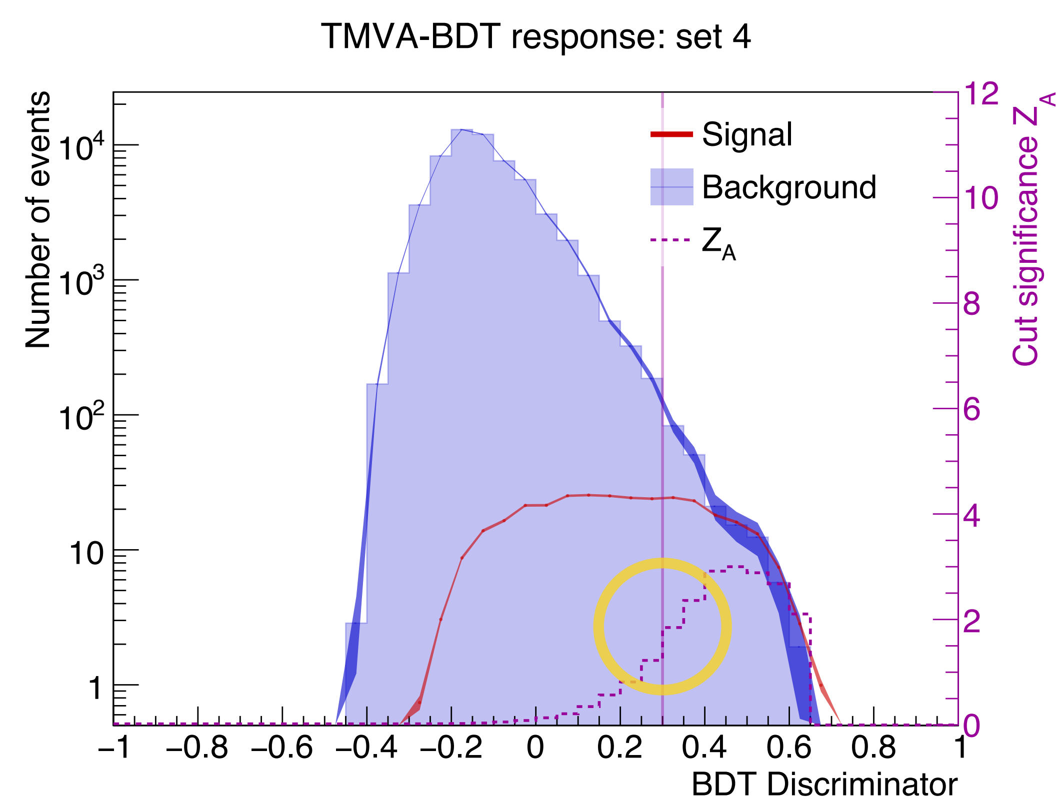
Sahin et al DOI:10.1016/j.nima.2016.09.017

Case Study II: Classifier Responses





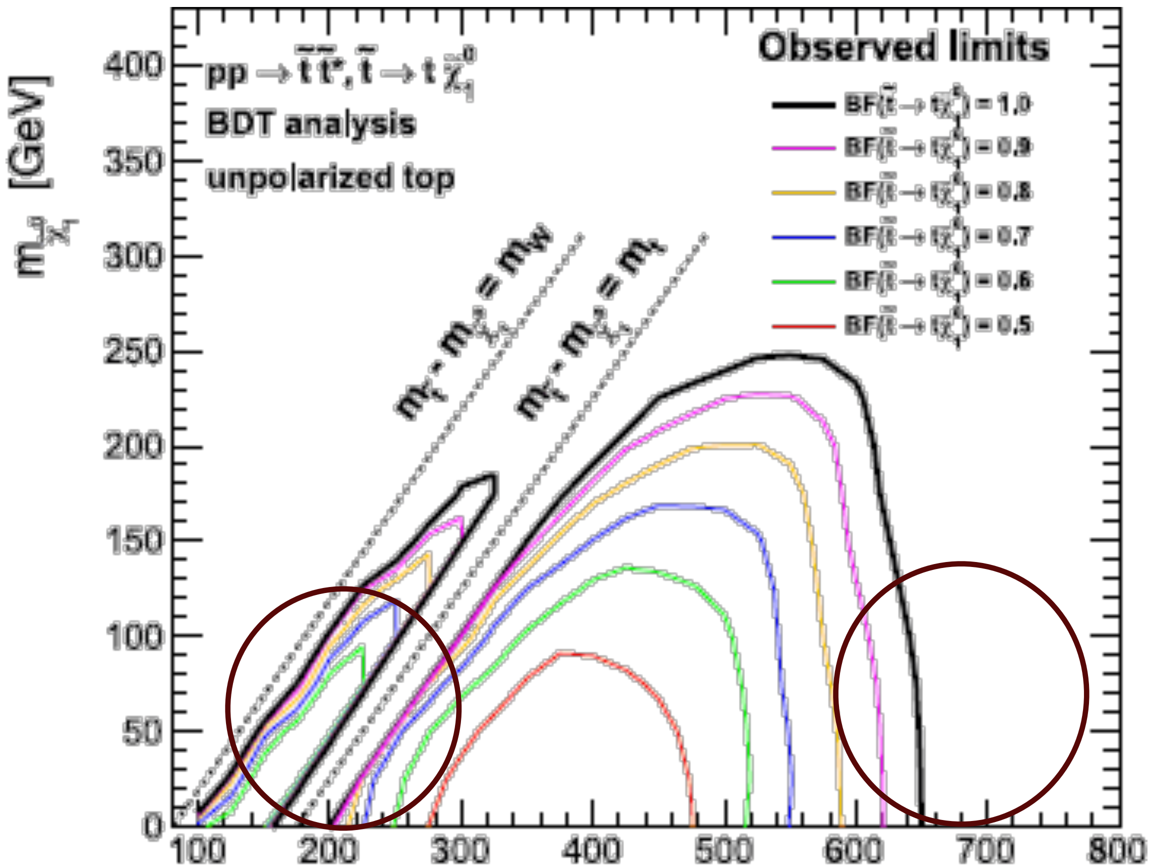




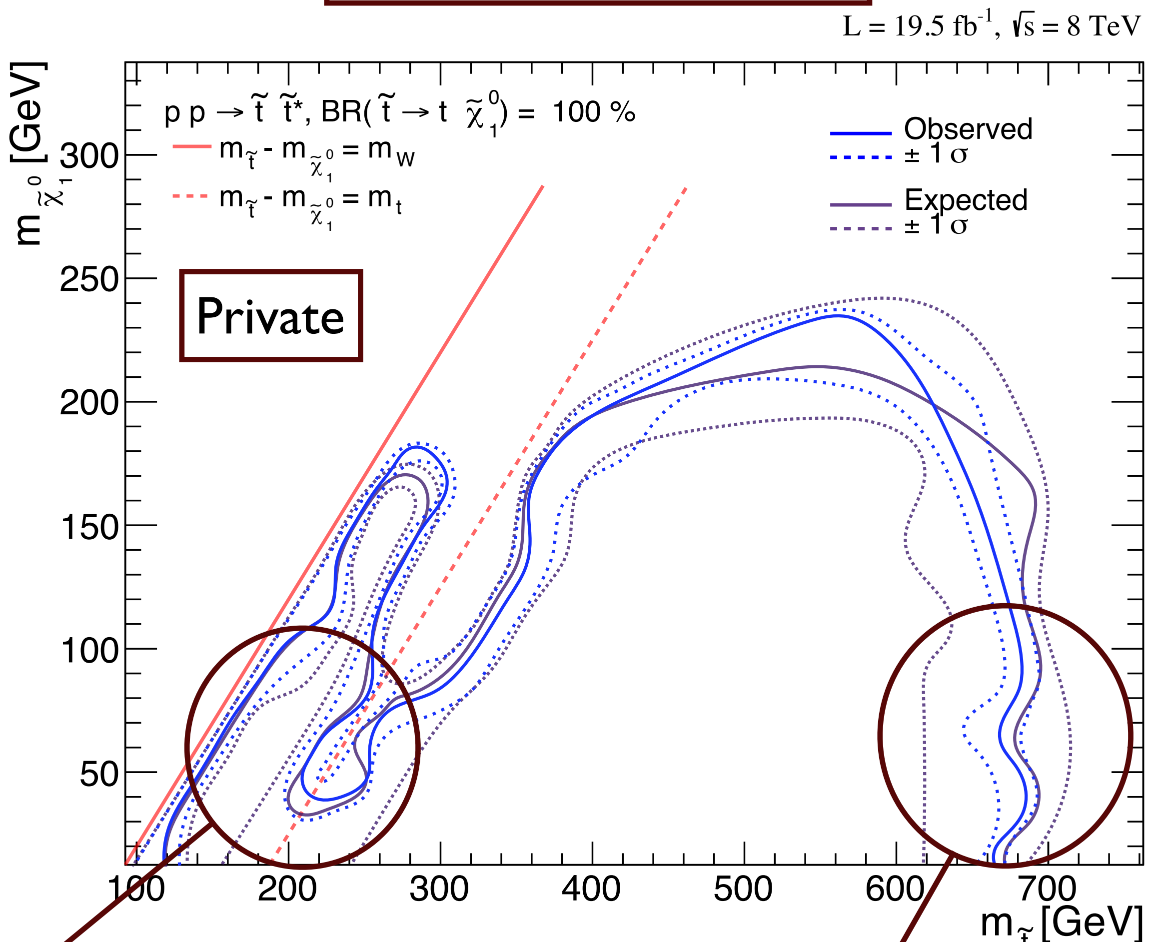
Both SVM-HINT and TMVA-BDT benefit from high number of variables.

Comparison of the results

CMS Col., EPJ C 73 (2013) 2677



DESY-THESIS-2017-014



- Improvement in the **compressed region** and in the **high top-squark mass**.

Conclusion

- A range of machine learning algorithms is widely employed in collider physics.
  - IMHO, we are still not at the front-line…
  - The possibilities are vast, but the support is limited. I hope collaborations with other disciplines also help people to realize the importance.
- As an unsupervised learning algorithm DBSCAN clustering algorithm is presented. DBSCAN is proven to be fast, flexible and resilient against possible noise.
  - DBSCAN seems to perform better under high-PU.
- An SVM interface for the HEP data classification problems using a statistical significance (Asimov Significance estimator) based hyperparameter optimization is presented. Available on Github:
  - https://github.com/ml-hint/svm-hint
  - The implementation provides a strong classification out of the box with a built-in autonomous optimization.

thank you!

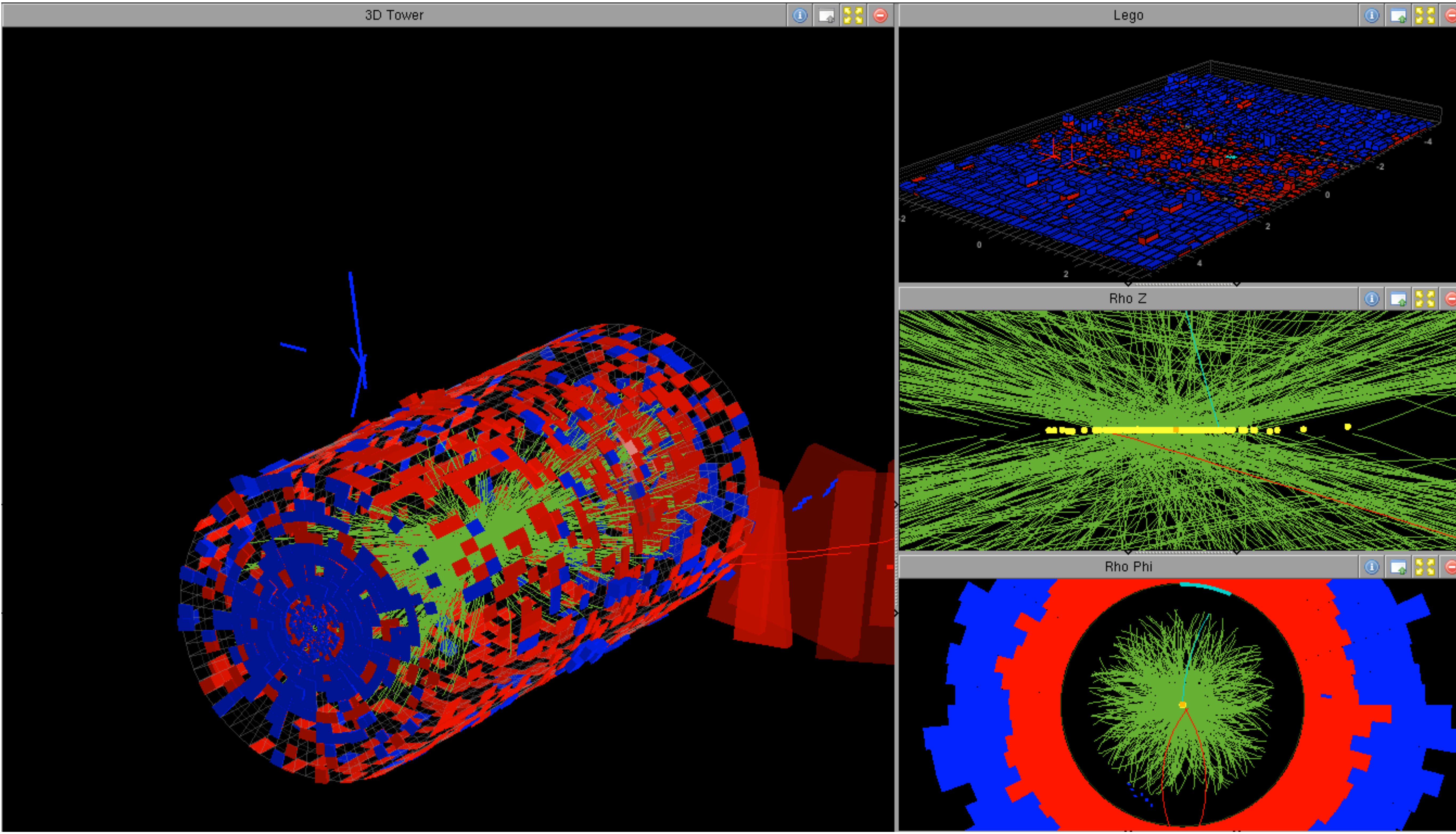
References

References

- TMVA Package (a complete and easy to use HEP - ML software) built in to the ROOT framework (a C++ based CERN - Fermilab developed analysis framework for Big Data analysis):
  - TMVA: https://github.com/root-project/root/tree/master/tmva
  - ROOT:https://github.com/root-project/root/
- Some books for interested (the first book is more of the fundamentals the second book is related to Deep Learning which is not covered in this talk):
  - https://www.amazon.com/Pattern-Recognition-Learning-Information-Statistics/dp/0387310738
  - https://www.amazon.com/Deep-Learning-Adaptive-Computation-Machine/dp/0262035618/
- Cowan et al (Asimov Paper) Eur. Phys. J .C71:1554, 2011
- Sahin et al (SVM-HINT paper) DOI:10.1016/j.nima.2016.09.017

Backup

CMS event display



Asimov Significance

$$Z_A = \left[2\left((s+b)\ln\left[\frac{(s+b)(b+\sigma_b^1)}{b^2+(s+b)\sigma_b^2}\right] - \frac{b^2}{\sigma_b^2}\ln\left[1+\frac{\sigma_b^2 s}{b(b+\sigma_b^2)}\right]\right)\right]^{1/2}$$

- http://www.pp.rhul.ac.uk/~cowan/atlas/cowan_atlas_15feb11,
  - * Eur. Phys. J .C71:1554, 2011.
- Gives a very close estimation of the quoted significances.

$\hat{\mu}_b$	1.3	3.8	3.8	388.6	493434	2109732
$s = n - \hat{\mu}_b$	4.7	5.2	13.2	134	4992	9717
$f = \sigma_b/\hat{\mu}_b$	0.231	0.237	0.158	0.0207	0.00142	0.000206
Quoted Z	2.7	1.9	4.6	5.9	5.0	6.4
Z_A	2.8	2.0	4.6	5.9	5.0	6.4