Fisher information metrics for binary classifier evaluation and training

Event selection for HEP precision measurements

Andrea Valassi
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CHEP 2018, Sofia – Machine Learning and Physics Analysis session

Why and when I got interested in this topic

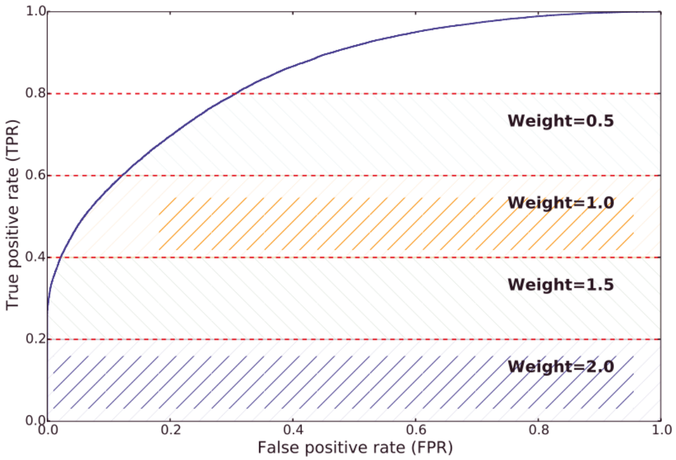


Figure 3: Weights assigned to the different segments of the ROC curve for the purpose of submission evaluation. The x axis is the False Positive Rate (FPR), while the y axis is True Positive Rate (TPR).

T. Blake at al., *Flavours of Physics: the machine learning challenge for the search of $\tau \to \mu\mu\mu$ decays at LHCb* (2015, unpublished). https://kaggle2.blob.core.windows.net/competitions/kaggle/4488/media/lhcb_description_official.pdf (accessed 15 January 2018)

The 2015 LHCb Kaggle ML Challenge:
- Develop an event selection in a search for $\tau \to \mu\mu\mu$

ML binary classifier problem
- *Evaluation: the highest weighted AUC is the winner*

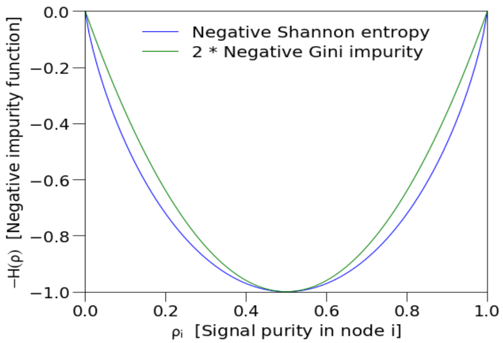
- First time I saw an *Area Under the Roc Curve (AUC)*
- My reaction:
  – What is the AUC? Which other scientific domains use it and why?
  – *Is the AUC relevant in HEP? Can we develop HEP-specific metrics?*

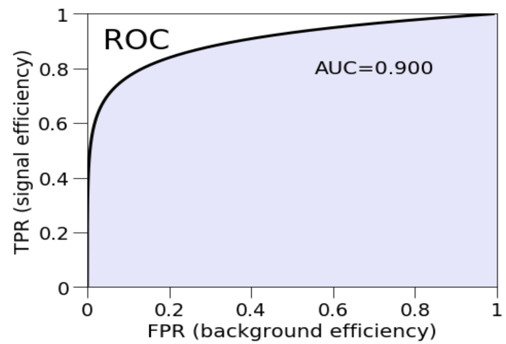
Overview – the scope of this talk

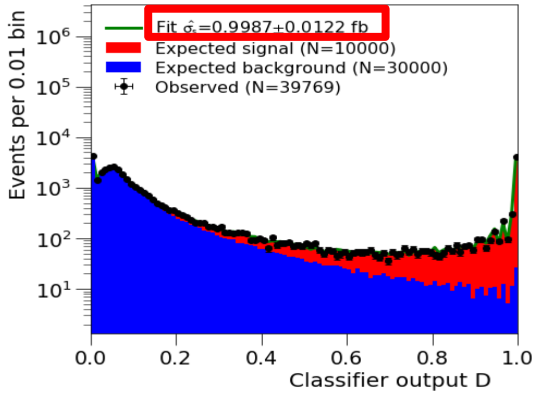
- *Different domains and/or problems → Need different metrics*
  - Always keep your final goal in mind
- Focus on a specific HEP example: *event selection to minimize statistical error $\Delta\theta$ in an analysis for the point estimation of θ*
  - Do not focus on: tracking, systematic errors, trigger, searches…
- *Whenever you take a decision, base it on the minimization of $\Delta\theta$*
  - Metrics for physics precision → final goal: minimize $\Delta\theta$
  - Metrics for binary classifier evaluation → (is the AUC relevant?)
  - Metrics for binary classifier training → (are standard ML metrics relevant?)

Training, Evaluation, Physics: one metric to bind them all?

Example: event selection using a Decision Tree for a parameter fit







TRAINING

- (either) **Gini impurity**
  - *Economics: inequality*
  - *Ecology: diversity*
- (or) **Shannon information**
  - *Information theory: entropy*

EVALUATION

- **ROC Curve** **(Receiver Operating Characteristic)**
  - *Signal detection: radar detection*
  - *Psychophysics: sensory detection*
- **AUC (Area Under the ROC Curve)**
  - *Radiology, Medicine: diagnostic accuracy*

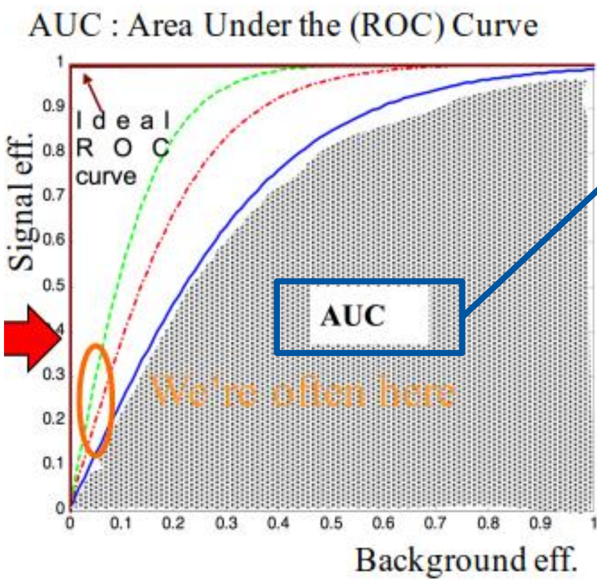
PHYSICS

- **Precision**
  - *Parameter estimation: measurement error $\Delta\theta$*

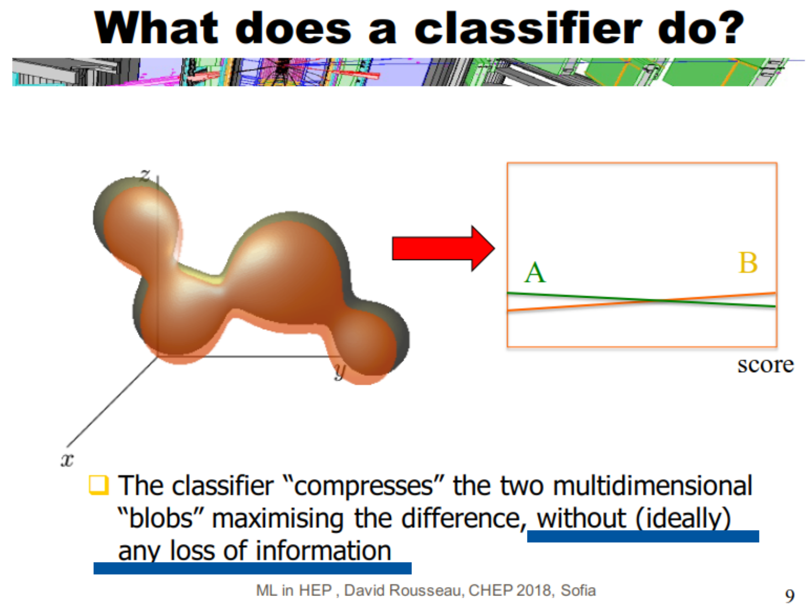
Proposal: use metrics based on Fisher Information in all three steps

(Fisher Information about θ ~is $I_\theta = 1/(\Delta\theta)^2$ – maximize I_θ to minimize $\Delta\theta$)

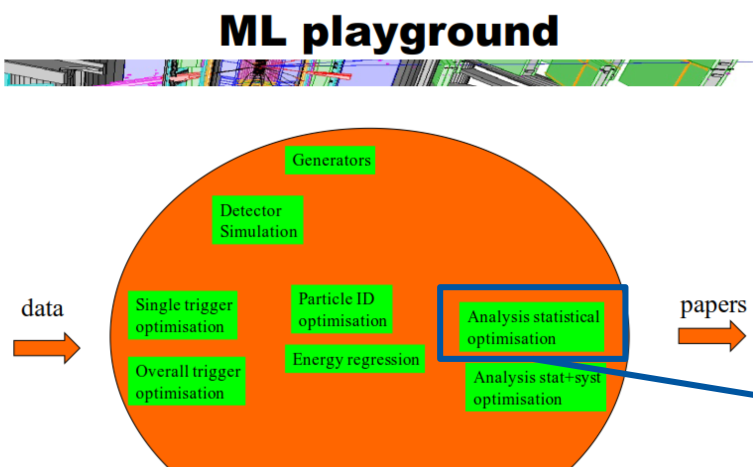
CHEP plenary this morning



I will argue against AUC's for evaluation in HEP



I will discuss the retention of *Fisher* information in classifiers



I will describe one problem in analysis statistical optimization

Binary classifier evaluation – reminder

Discrete classifiers: the confusion matrix

Binary decision:
signal or background

	true class: **P**ositives (HEP: **signal Stot**)	***true class***: **N**egatives (HEP: **background Btot**)
classified as: positives (HEP: **selected**)	**True Positives (TP)** (HEP: selected signal **Ssel**)	**False Positives (FP)** (HEP: selected bkg **Bsel**)
classified as: negatives (HEP: **rejected**)	**False Negatives (FN)** (HEP: rejected signal **Srej**)	**True Negatives (TN)** (HEP: rejected bkg **Brej**)

$$\mathrm{PPV} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FP}}$$

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}$$

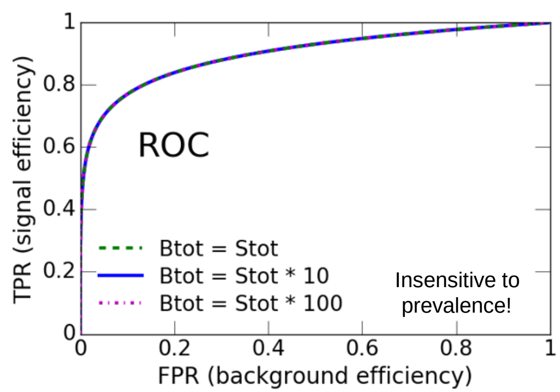
$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{TN}+\mathrm{FP}} = 1-\mathrm{FPR}$$

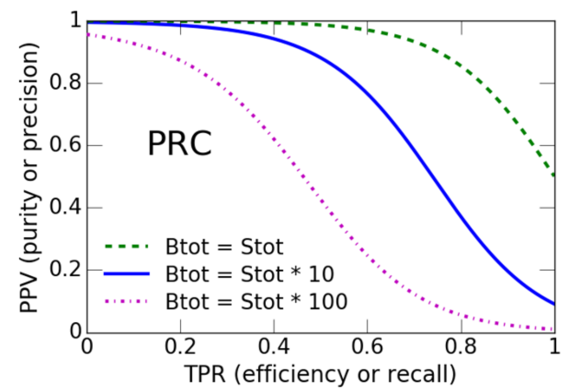
Prevalence $\pi_s = \frac{S_{\mathrm{tot}}}{S_{\mathrm{tot}}+B_{\mathrm{tot}}}$

Scoring classifiers: ROC and PRC curves

Continuous output:
probability to be signal

Vary the binary decision
by varying the cut
on the scoring classifier





Binary classifier evaluation in other domains

Medical Diagnostics (MD) $\rightarrow$ e.g. diagnostic accuracy for cancer

– *Symmetric: all patients important, both truly ill (TP) and truly healthy (TN)*
– ROC-based analysis (because ROC insensitive to prevalence)
  - *AUC interpretation: probability that diagnosis gives greater suspicion to a randomly chosen sick subject than to a randomly chosen healthy subject*

Information Retrieval (IR) $\rightarrow$ e.g. find pages in Google search

– *Asymmetric: distinction between relevant and non-relevant documents*
– PRC-based evaluation: precision and recall (= purity and efficiency in HEP)
  - Single metric: e.g. Mean Average Precision ~ area under PRC (AUCPR)

Oversimplification: $\boxed{\mathrm{AUC} = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s}$ (MD) vs. (IR) $\boxed{\mathrm{AUCPR} = \int_0^1 \rho \, d\epsilon_s}$

Evaluation: (main) specificities of HEP

1. Qualitative asymmetry: signal interesting, background irrelevant
   – Like Information Retrieval: use purity and efficiency (precision and recall)
     • *True Negatives and the AUC are irrelevant in HEP event selection*

2. Distribution fits: several disjoint bins, not just a global selection
   – Analyze *local signal efficiency and purity in each bin*, not just global ones
   – Frequent special case: fits involving distributions of the scoring classifier

3. Signal events not all equal: they may have different sensitivities
   – Example: only events close to a mass peak are sensitive to the mass

Illustrated in the following by three examples (1=FIP1, 1+2=FIP2, 1+2+3=FIP3)

Evaluation: Fisher Information Part (FIP)

- Evaluation of an event selection from its effect on the error $\Delta\hat{\theta}$
  - *Compare to "ideal" case where there is no background*

- FIP: fraction of "ideal" FI that is retained by the real classifier
  - Range in [0,1] $\rightarrow$ 0 if no signal, 1 if select all signal and no background
  - Qualitatively relevant: higher is better $\rightarrow$ maximize FIP to minimize $\Delta\hat{\theta}$
  - Numerically meaningful: related to $\Delta\hat{\theta}$

- For a binned fit of θ from a (1-D or multi-D) histogram:
  - Consider only statistical errors $\rightarrow$ sum information from the different bins

$$\mathrm{FIP} = \frac{\mathcal{I}_\theta^{(\mathrm{real\ \ classifier})}}{\mathcal{I}_\theta^{(\mathrm{ideal\ \ classifier})}} = \frac{\sum_{i=1}^{m} \epsilon_i \rho_i \times \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}{\sum_{i=1}^{m} \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}$$

Remember from the previous slide:
1. Qualitative asymmetry: use ε and ρ (as in IR)
2. Distribution fit: need local ε_i and ρ_i in each bin
3. Signal events not all equal: need sensitivity $\frac{1}{S_i}\frac{\partial S_i}{\partial \theta}$

[FIP1] Cross-section in counting experiment

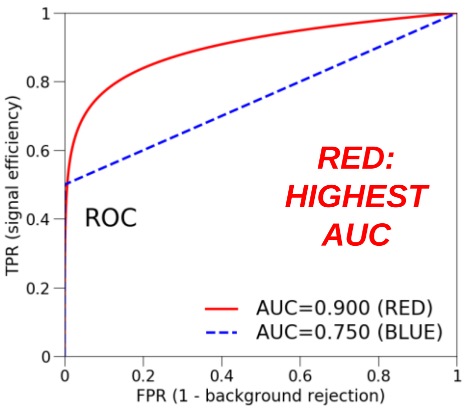
- Counting experiment: measure a single number N_{meas}
  - Well-known since decades: maximize $\varepsilon_s * \rho$ to minimize statistical errors

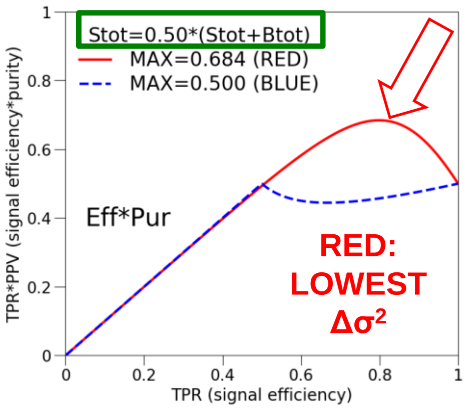
- FIP special case:
  - Counting experiment (1 bin) → *global* signal efficiency and purity
  - *Cross-section fit $\theta=\sigma_s$ → all events have equal sensitivity* $\frac{1}{S_i}\frac{\partial S_i}{\partial \sigma_s} = \frac{1}{\sigma_s}$

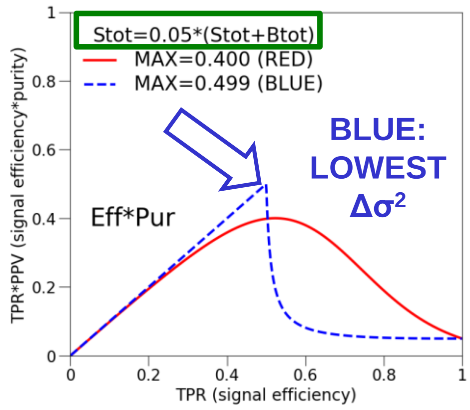
$$\mathrm{FIP} = \frac{\mathcal{I}_\theta^{(\text{real classifier})}}{\mathcal{I}_\theta^{(\text{ideal classifier})}} = \frac{\sum_{i=1}^{m} \epsilon_i \rho_i \times \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}{\sum_{i=1}^{m} \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2} \rightarrow \boxed{\mathrm{FIP1} = \varepsilon_s * \rho}$$

Examples of issues in AUCs – *crossing ROCs*

- Cross-section measurement by counting experiment
  - Maximize FIP1=ε_s*ρ → Minimize the statistical error $\Delta\sigma^2$
- Compare two classifiers: red (AUC=0.90) and blue (AUC=0.75)
  - The red and blue ROCs cross (otherwise the choice would be obvious!)
- Choice of classifier achieving minimum $\Delta\sigma^2$ *depends on S_{tot}/B_{tot}*
  - *Signal prevalence 50%*: choose classifier with higher AUC (red)
  - *Signal prevalence 5%*: choose classifier with lower AUC (blue)
  - AUC is irrelevant – and ROC is only useful if you also know prevalence







	FIP1	AUC
Range in [0,1]	YES	YES
Higher is better	YES	NO
Numerically meanigful	YES	NO

Optimal partitioning in distribution fits

- Does information I_θ increase if I split a bin into two ($n \rightarrow n_L+n_R$)?
  - Information gain is $\Delta I_\theta = \left(\rho_L \frac{1}{s_L}\frac{\partial s_L}{\partial\theta} - \rho_R \frac{1}{s_R}\frac{\partial s_R}{\partial\theta}\right)^2 * \frac{n_L n_R}{n_L+n_R}$

- Partition events using optimal binning variables (→ two examples)
  - For cross-sections $\left(\frac{1}{s_i}\frac{\partial s_i}{\partial\sigma_s} = \frac{1}{\sigma_s}\right)$: *separate bins with different ρ_i* (→"FIP2")
  - For a generic parameter θ : *separate bins with different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial\theta}$* (→"FIP3")

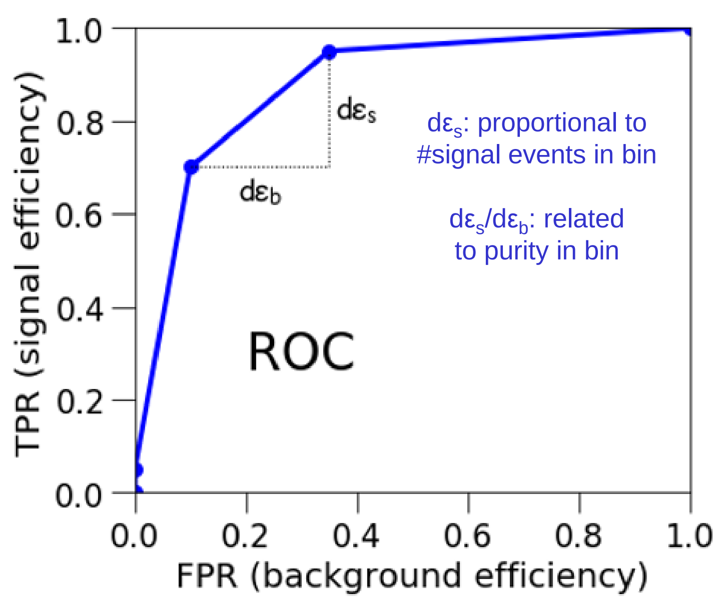
- Practical ML consequences (focus on cross-section example):
  - *Use the scoring classifier (i.e. ~ρ !) to partition events, not to reject them*
  - *Train the scoring classifier to maximize the total Fisher information* of the histogram binning, i.e. train it to maximize its partitioning power
    - Use Fisher Information as a node splitting criterion for decision tree training
    - *Use the decision tree more as a regression tree than as a classification tree*

[FIP2] cross-section fit on the 1-D scoring classifier distribution – evaluation

- FIP special case
  - Cross-section: constant $\frac{1}{s_i}\frac{\partial s_i}{\partial \sigma_s} = \frac{1}{\sigma_s}$
  - Fit on all events: ε_i=1 in all bins
  - Fit scoring classifier: use ROC *and prevalence* to determine purity ρ_i
    - Region of constant ROC slope is a region of constant signal purity

$$\mathrm{FIP2} = \int_0^1 \frac{d\epsilon_s}{1 + \frac{1-\pi_s}{\pi_s}\frac{d\epsilon_b}{d\epsilon_s}}$$

Compare FIP2 to AUC: $\mathrm{AUC} = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s$

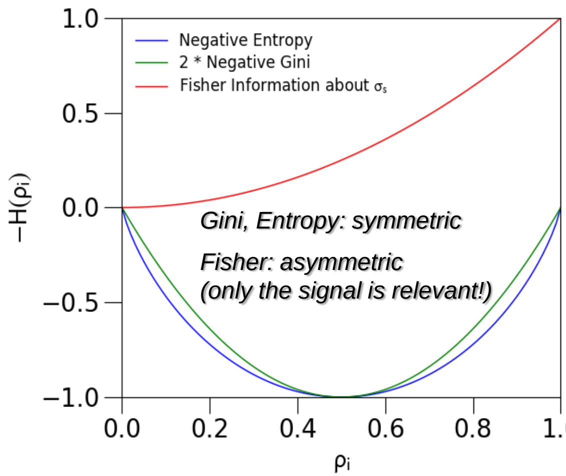


[FIP2] cross-section fit on the 1-D scoring classifier distribution – training

- Is there a gain if I split a node into two ($n \rightarrow n_L+n_R$)?
  - Same question as in optimal partitioning: do I gain by splitting a bin?
- Gain depends on "impurity" function H(ρ): $\Delta = -n_L H(\rho_L) - n_R H(\rho_R) + n H(\rho)$
  - two standard choices: Shannon information (entropy) and Gini impurity
  - *I suggest a third option: Fisher information I_{σ_s} about the cross-section σ_s*
- Surprise: different functions, but *Gini and Fisher gains are equal!*

$$\Delta_{\text{Fisher}} = \frac{(s_L n_R - s_R n_L)^2}{n_L n_R (n_L + n_R)} = \frac{\Delta_{\text{Gini}}}{2}$$

  - So, Gini is OK for cross-sections (or searches?)
  - *But more intuitive physics interpretation for Fisher*
  - No practical gain here, but important principle
    - And proof-of-concept for generic parameter θ



[FIP3] generic parameter fits including the scoring classifier distribution – *work in progress*

- Not a cross-section, e.g. a coupling fit: signal events not all equal
  - –[FIP2] Fit for $\sigma_s \rightarrow$ should partition events into bins with different ρ_i
  - –[FIP3] Fit for θ $\rightarrow$ should partition events into bins with different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial\theta}$

- Example: 2-D fit for θ of the ρ and $\frac{1}{s}\frac{\partial s}{\partial\theta}$ distributions
  - –Train a *regression tree for* $\frac{1}{s}\frac{\partial s}{\partial\theta}$ (on MC weight derivative) using signal alone
  - –Train a *regression tree for ρ* using signal (weighted by $\frac{1}{s}\frac{\partial s}{\partial\theta}$) and background
  - –Use Fisher Information about θ as the gain function in both cases

Boundary between classification and regression even more blurred

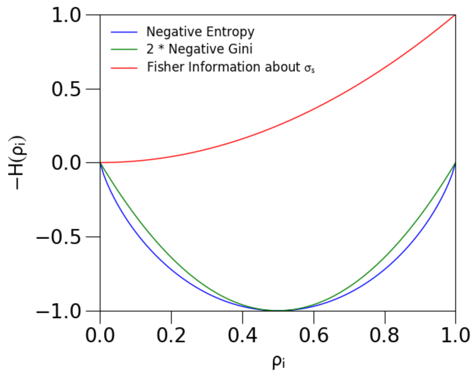
Software technicalities

- I use Python (SciPy, iminuit, bits of rootpy) on SWAN at CERN
  - Thanks to all involved in these projects!
- Custom impurity not available in sklearn DecisionTree's
  - Planned for future sklearn releases (issue #10251 and MR #10325)?
  - I implemented a very simple DecisionTree from scratch, starting from the excellent iCSC notebooks by Thomas Keck (thanks!)
- I plan to make the software available when I find the time…

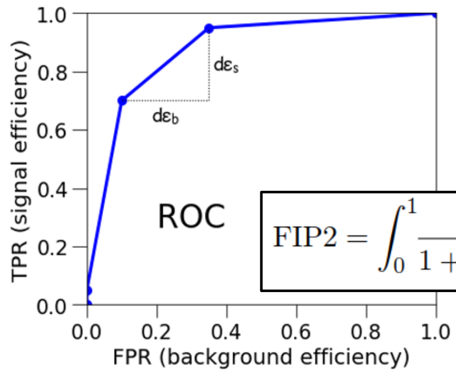
Conclusions and outlook

A paper will be on arxiv soon with all details

- Fisher Information: one metric to bind them all

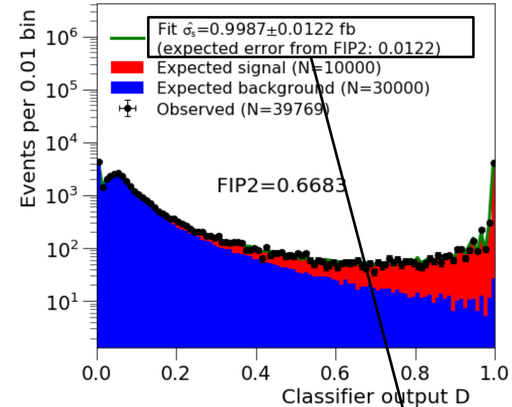


TRAINING
- Fisher Information
  = *measurement error*



$$\mathrm{FIP2} = \int_0^1 \frac{d\epsilon_s}{1 + \frac{1-\pi_s}{\pi_s}\frac{d\epsilon_b}{d\epsilon_s}}$$

EVALUATION
- Fisher Information
  = *measurement error*



PHYSICS
- Fisher Information
  = *measurement error*

- Use scoring classifiers to partition events, not to reject them
  - The boundary between classification and regression is blurred

- We must and can define our own HEP specific metrics
  - I described one case, there are others (searches, systematics, tracking...)
  - Focus on signal. Describe distribution fits. Signal events are not all equal.
  - *Can we please stop using the AUC now?* ☺

Backup slides

Backup – statistical error in binned fits

- Data: *observed event counts n_i* in m bins of a (multi-D) distribution f(x)
  - *expected event counts y_i* = $f(x_i,\theta)dx$ depend on a parameter θ that we want to fit
  - [NB here f is a differential cross section, it is not normalized to 1 like a pdf]

- Fitting θ is like combining the independent measurements in the m bins
  - expected error on n_i in bin x_i is $\Delta n_i = \sqrt{y_i} = \sqrt{f(xi,\theta)\,dx}$
  - expected error on $f(x_i,\theta)$ in bin x_i is $\Delta f = f * \Delta n_i/n_i = \sqrt{f / dx}$
  - expected error on estimated $\hat{\theta}_i$ in bin x_i is $\frac{1}{(\Delta\hat{\theta})^2_{(\mathrm{bin}\ dx)}} = \left(\frac{\partial f}{\partial\theta}\right)^2 \frac{1}{(\Delta f)^2} = \left(\frac{\partial f}{\partial\theta}\right)^2 \left(\frac{\sqrt{dx}}{\sqrt{f}}\right)^2 = \left(\frac{\partial f}{\partial\theta}\right)^2 \frac{dx}{f}$
  - expected error on estimated $\hat{\theta}$ by combining the m bins is $\left(\frac{1}{\Delta\hat{\theta}}\right)^2 = \int \frac{1}{f}\left(\frac{\partial f}{\partial\theta}\right)^2 dx$

- A bit more formally, joint probability for observing the n_i is $P(\mathbf{n};\theta) = \prod_{i=1}^{m} \frac{e^{-y_i} y_i^{n_i}}{n_i!}$
  - Fisher information on θ from the data available is then

$$\mathcal{I}_\theta = E\left[\frac{\partial \log P(\mathbf{n};\theta)}{\partial\theta}\right]^2 \quad \text{i.e.} \quad \mathcal{I}_\theta = \sum_{i=1}^{m} \frac{1}{y_i}\left(\frac{\partial y_i}{\partial\theta}\right)^2 = \int \frac{1}{f}\left(\frac{\partial f}{\partial\theta}\right)^2 dx$$

  - The minimum variance achievable (Cramer-Rao lower bound) is $(\Delta\hat{\theta})^2 = \mathrm{var}(\hat{\theta}) \geq \frac{1}{\mathcal{I}_\theta}$

Optimal partitioning – information inflow

- Information about θ in a binned fit → $\mathcal{I}_\theta = \sum_{i=1}^{m} \frac{1}{y_i} \left(\frac{\partial y_i}{\partial \theta} \right)^2$
- Can I reduce $\Delta\hat{\theta}$ by splitting bin y_i into two bins? $y_i = w_i + z_i$
  - Is the "information inflow" positive? $\frac{1}{w_i}\left(\frac{\partial w_i}{\partial \theta}\right)^2 + \frac{1}{z_i}\left(\frac{\partial z_i}{\partial \theta}\right)^2 - \frac{1}{w_i+z_i}\left(\frac{\partial (w_i+z_i)}{\partial \theta}\right)^2 = \frac{\left(w_i \frac{\partial z_i}{\partial \theta} - z_i \frac{\partial w_i}{\partial \theta}\right)^2}{w_i z_i (w_i+z_i)} \geq 0$
  - information increases (error $\Delta\hat{\theta}$ decreases) if $\frac{1}{w_i}\frac{\partial w_i}{\partial \theta} \neq \frac{1}{z_i}\frac{\partial z_i}{\partial \theta}$
- In the presence of background: $\frac{1}{y_i}\frac{\partial y_i}{\partial \theta} = \rho_i \frac{1}{S_i}\frac{\partial S_i}{\partial \theta}$
  - information increases if $\rho_w \frac{1}{s_w}\frac{\partial s_w}{\partial \theta} \neq \rho_z \frac{1}{s_z}\frac{\partial s_z}{\partial \theta}$
  - therefore: **try to partition the data into bins of different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$**
    - for cross-section measurements, $\frac{1}{S_i}\frac{\partial S_i}{\partial \sigma_s} = \frac{1}{\sigma_s}$: *split into bins of different ρ_i*
- Two important practical consequences:
  - *1. use scoring classifiers to partition the data, not to reject events*
  - *2. information can be used also for training classifiers like decision trees*

More detailed slides

(Draft uploaded on July 2nd)

CHEP 2018
Sofia, Bulgaria

Draft uploaded on July 2nd

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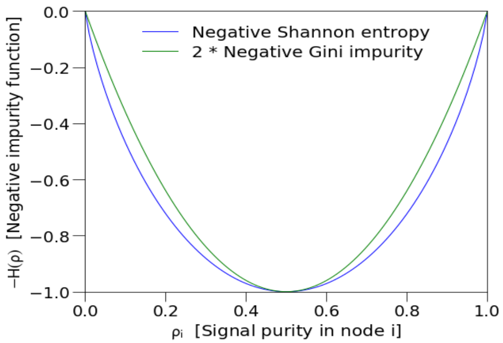
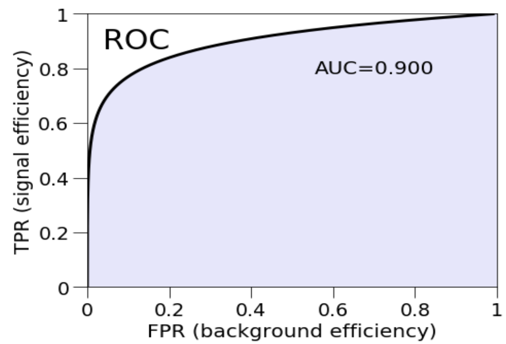
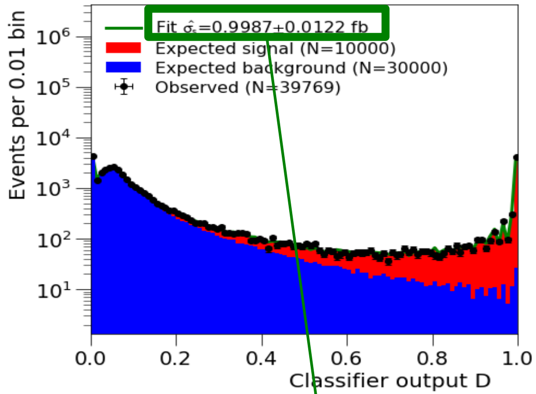
Training, Evaluation, Physics: one metric to bind them all?

An <u>oversimplified example</u>: Decision Tree for a cross-section fit







TRAINING
- (either) **Gini impurity**
  - *Economics: inequality*
  - *Ecology: diversity*
- (or) **Shannon information**
  - *Information theory: entropy*

EVALUATION
- **ROC Curve (Receiver Operating Characteristic)**
  - *Signal detection: radar detection*
  - *Psychophysics: sensory detection*
- **AUC (Area Under the ROC Curve)**
  - *Radiology, Medicine: diagnostic accuracy*

PHYSICS
- **Precision**
  - *Parameter estimation:* ***measurement error***

Different problems need different metrics → Always keep the final goal in mind!

<u>Main idea of this talk: use physics precision (Fisher information) also for evaluation and training: MINIMIZE MEASUREMENT ERRORS!</u>

Limited scope of this talk

- Different problems *also within HEP* require different metrics

- In this talk, I will focus on one specific problem:
  - Optimize event selection to minimize statistical errors in point estimation

- Three specific examples (I will focus on the second one)
  - [FIP1] *Total cross-section* measurement in a *counting experiment*
  - [FIP2] *Total cross-section* measurement by *distribution fit*
  - [FIP3] *Generic model parameter fit* (e.g. mass/coupling) by *distribution fit*
    - Even more specific: FIP2 and FIP3 use fits of the scoring classifier distribution

Binary classifier evaluation – reminder

Discrete classifiers: the confusion matrix

Binary decision: signal or background

	true class: **P**ositives (HEP: **signal Stot**)	*true class*: **N**egatives (HEP: **background Btot**)
classified as **P**ositives (HEP: **selected**)	**True Positives (TP)** (HEP: selected signal **Ssel**)	**False Positives (FP)** (HEP: selected bkg **Bsel**)
classified as **N**egatives (HEP: **rejected**)	**False Negatives (FN)** (HEP: rejected signal **Srej**)	**True Negatives (TN)** (HEP: rejected bkg **Brej**)

TP (S_{sel}) FP (B_{sel}) **FN** (S_{rej}) TN (B_{rej})	**TP** (S_{sel}) **FP** (B_{sel}) FN (S_{rej}) TN (B_{rej})	TP (S_{sel}) **FP** (B_{sel}) FN (S_{rej}) **TN** (B_{rej})
$\mathbf{TPR} = \frac{\mathbf{TP}}{\mathbf{TP}+\mathbf{FN}}$	$\mathbf{PPV} = \frac{\mathbf{TP}}{\mathbf{TP}+\mathbf{FP}}$	$\mathbf{TNR} = \frac{\mathbf{TN}}{\mathbf{TN}+\mathbf{FP}} = \mathbf{1}-\mathbf{FPR}$
HEP: "efficiency" $\epsilon_s = \frac{S_{sel}}{S_{tot}}$	HEP: "purity" $\rho = \frac{S_{sel}}{S_{sel}+B_{sel}}$	HEP: "background rejection" $1-\epsilon_b = 1-\frac{B_{sel}}{B_{tot}}$
IR: "recall"	IR: "precision"	—
MED: "sensitivity"	—	MED: "specificity"

Different domains
→ Focus on different concepts
→ Use different terminologies

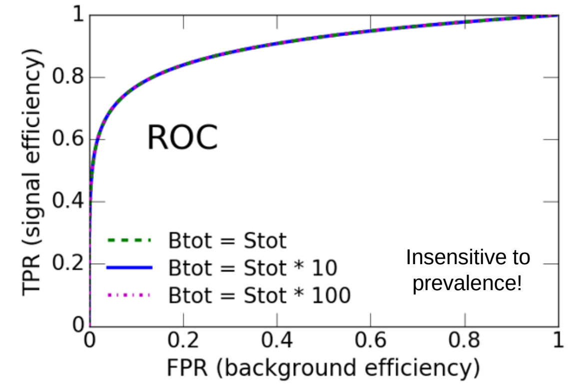
Examples from three domains:
- **Medical Diagnostics (MED)**
  does Mr. A. have cancer?
- **Information Retrieval (IR)**
  Google documents about "ROC"
- **HEP event selection (HEP)**
  select Higgs event candidates

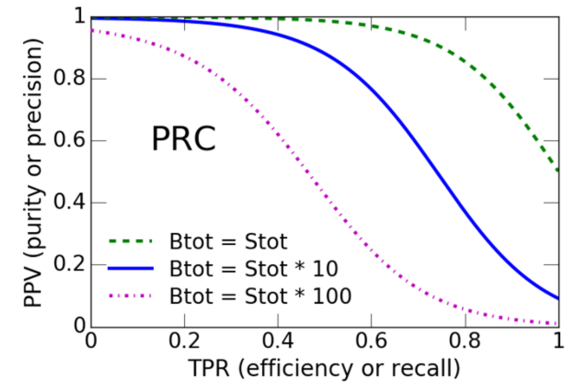
MED: prevalence
$$\pi_s = \frac{S_{tot}}{S_{tot}+B_{tot}}$$

Scoring classifiers: ROC and PRC curves

Continuous output: probability to be signal

Vary the binary decision by varying the cut on the scoring classifier





Binary classifier evaluation in other domains

Medical Diagnostics (MD) $\rightarrow$ diagnostic accuracy

- <u>*Symmetric: all patients important, both truly ill (TP) and truly healthy (TN)*</u>
- Traditional $\mathrm{ACC} = \frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}$ was too sensitive to prevalence: moved to ROC
  - But now ROC is questioned as too insensitive to prevalence (imbalanced data)
- ROC-based analysis: sensitivity and specificity
  - Accuracy metric: e.g. *AUC = probability that diagnosis gives greater suspicion to a randomly chosen sick subject than to a randomly chosen healthy subject*

Information Retrieval (IR)

- <u>*Asymmetric: distinction between relevant and non-relevant documents*</u>
- PRC-based evaluation: precision and recall
  - Single metric: e.g. Mean Average Precision ~ area under PRC (AUCPR)

Oversimplification: $\mathrm{AUC} = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s$ (MD) vs. (IR) $\mathrm{AUCPR} = \int_0^1 \rho \, d\epsilon_s$

Evaluation: (main) specificities of HEP

1. Qualitative asymmetry: only the signal has interesting physics

- HEP event selection is like Information Retrieval: background is irrelevant
  - *True Negatives and the AUC are irrelevant in HEP event selection*
- Classical evaluation metrics: signal efficiency and purity (the PRC in IR!)
  - *ROC alone is not enough – also need prevalence to interpret the ROC*

2. Distribution fits: several disjoint bins, not just a global selection

- Analyze *local signal efficiency and purity in each bin*, not just global ones
- Counting experiments (e.g. FIP1) vs. distribution fits (e.g. FIP2, FIP3)
  - Special case: fits involving distributions of the scoring classifiers

3. Signal events not all equal: they *may* have different sensitivities

- Example: only events close to a mass peak are sensitive to the mass
- Total cross-section (e.g. FIP1, FIP2) vs. generic parameter fit (e.g. FIP3)

Fisher Information Part (FIP)

- Consider a measurement $\hat{\theta}$ of one physics parameter θ
  - Fisher Information about θ is $1/\Delta\hat{\theta}^2$ (keep this simple, not formal)

- Evaluate an event selection from the effect on the error $\Delta\hat{\theta}$
  - *Compare to an "ideal" case where there is no background*

- FIP: fraction of "ideal" FI that is retained by the real classifier
  - Range in [0,1] $\rightarrow$ 0 if no signal, 1 if select all signal and no background
  - Qualitatively relevant: higher is better $\rightarrow$ maximize FIP to minimize $\Delta\hat{\theta}$
  - Numerically meaningful: related to $\Delta\hat{\theta}$ $\rightarrow$ $(\Delta\hat{\theta}^{(\text{real classifier})})^2 = \frac{1}{\text{FIP}}(\Delta\hat{\theta}^{(\text{ideal classifier})})^2$

- For a binned fit of θ from a (1-D or multi-D) histogram:
  - With expected event counts in i^{th} bin $y_i = \epsilon_i{*}S_i + b_i = \epsilon_i{*}S_i / \rho_i$
  - Consider only statistical errors $\rightarrow$ sum information from the different bins

$$\text{FIP} = \frac{\mathcal{I}_\theta^{(\text{real classifier})}}{\mathcal{I}_\theta^{(\text{ideal classifier})}} = \frac{\sum_{i=1}^{m} \epsilon_i \rho_i \times \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}{\sum_{i=1}^{m} \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}$$

Remember from the previous slide:
1. Only signal is interesting: background appears via ρ_i
2. Distribution fit: need local ϵ_i and ρ_i
3. Signal events are not all equal: need sensitivity $\frac{1}{S_i}\frac{\partial S_i}{\partial \theta}$

[FIP1] Cross-section in counting experiment

- Counting experiment: measure a single number N_{meas}
  - Well-known since decades: maximize ε_s*ρ to minimize statistical errors

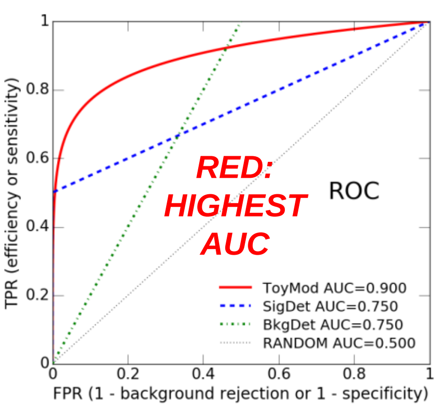
$$(\sigma_s)_{\rm meas} = \frac{N_{\rm meas} - \mathcal{L}\epsilon_b\sigma_b}{\mathcal{L}\epsilon_s} \quad \rightarrow \quad \frac{1}{(\Delta\sigma_s)^2} = \frac{1}{\sigma_s}\mathcal{L}\epsilon_s\rho = \frac{1}{\sigma_s^2}S_{\rm tot}\epsilon_s\rho = \frac{1}{\sigma_s^2}\times\frac{S_{\rm sel}^2}{S_{\rm sel}+B_{\rm sel}}$$

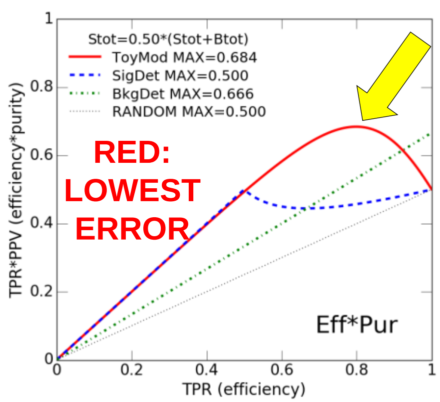
- FIP special case: FIP1 = ε_s*ρ
  - Counting experiment → global signal efficiency and purity
  - Cross-section fit $\theta=\sigma_s$ → all events have equal sensitivity $\frac{1}{S_i}\frac{\partial S_i}{\partial\sigma_s} = \frac{1}{\sigma_s}$

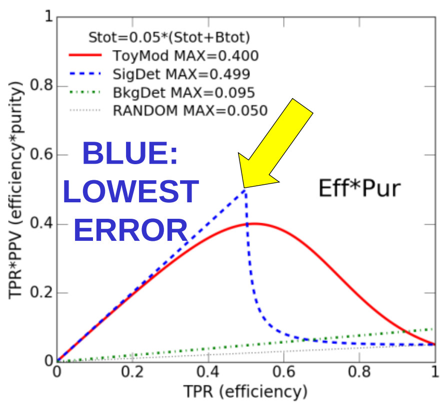
$$\mathrm{FIP} = \frac{\mathcal{I}_\theta^{(\rm real\ classifier)}}{\mathcal{I}_\theta^{(\rm ideal\ classifier)}} = \frac{\sum_{i=1}^{m}\epsilon_i\rho_i \times \frac{1}{S_i}\left(\frac{\partial S_i}{\partial\theta}\right)^2}{\sum_{i=1}^{m}\frac{1}{S_i}\left(\frac{\partial S_i}{\partial\theta}\right)^2} \quad \rightarrow \quad \boxed{\mathrm{FIP1} = \varepsilon_s*\rho}$$

Examples of issues in AUCs – crossing ROCs

- Cross-section measurement by counting experiment
  - maximize FIP1=ε_s*ρ → minimize the statistical error $\Delta\sigma^2$
- Compare two classifiers: red (AUC=0.90) and blue (AUC=0.75)
  - The red and blue ROCs cross (otherwise the choice would be obvious!)
- Choice of classifier achieving minimum $\Delta\sigma^2$ depends on S_{tot}/B_{tot}
  - Signal prevalence 50%: choose classifier with higher AUC (red)
  - Signal prevalence 5%: choose classifier with lower AUC (blue)
  - AUC is irrelevant – and ROC is only useful if you also know prevalence







	FIP1	AUC
Range in [0,1]	YES	YES
Higher is better	YES	NO
Numerically meanigful	YES	NO

Optimal partitioning – information inflow

- Does $\mathcal{I}_\theta = \sum_{i=1}^{m} \frac{1}{y_i} \left(\frac{\partial y_i}{\partial \theta} \right)^2$ increase if I split y_i into two bins? $y_i = w_i + z_i$
  - Information increases and error $\Delta\hat{\theta}$ decreases if $\frac{1}{w_i}\frac{\partial w_i}{\partial \theta} \neq \frac{1}{z_i}\frac{\partial z_i}{\partial \theta}$
  - In the presence of background, $\Delta\hat{\theta}$ decreases if $\rho_w \frac{1}{s_w}\frac{\partial s_w}{\partial \theta} \neq \rho_z \frac{1}{s_z}\frac{\partial s_z}{\partial \theta}$

- Hence: **try to partition the data into bins of different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$**
  - For cross-section measurements, $\frac{1}{S_i}\frac{\partial S_i}{\partial \sigma_s} = \frac{1}{\sigma_s}$: *split into bins of different ρ_i*
    - As the scoring classifier represents ρ, fit its distribution! (next slide: FIP2)

- Two important practical consequences:
  - *1. use scoring classifiers to partition the data, not to reject events*
  - *2. information can be used also for training classifiers like decision trees*

[FIP2] cross-section measurement by fitting the 1-D scoring classifier distribution

$$\text{FIP} = \frac{\mathcal{I}_\theta^{\text{(real classifier)}}}{\mathcal{I}_\theta^{\text{(ideal classifier)}}} = \frac{\sum_{i=1}^{m} \epsilon_i \rho_i \times \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}{\sum_{i=1}^{m} \frac{1}{S_i}\left(\frac{\partial S_i}{\partial \theta}\right)^2}$$

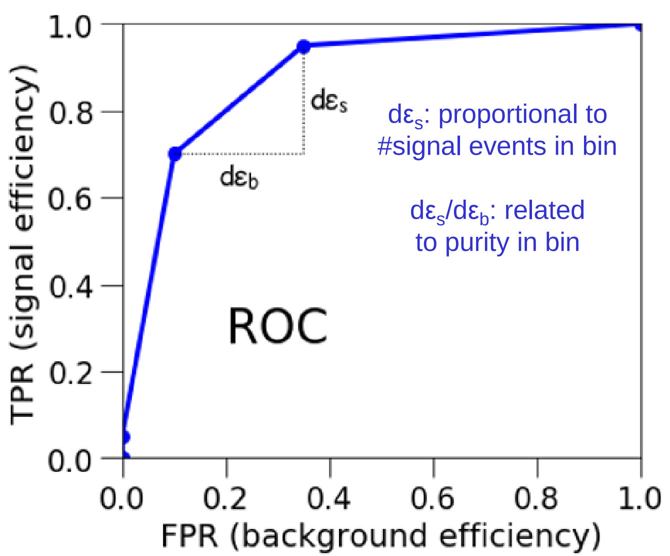
- FIP special case
  - Cross-section: constant $\frac{1}{s_i}\frac{\partial s_i}{\partial \sigma_s} = \frac{1}{\sigma_s}$
  - Fit on all events: ϵ_i=1 in all bins

  $\rightarrow$ $\text{FIP2} = \frac{\sum_{i=1}^m s_i^2/n_i}{\sum_{i=1}^m s_i} = \frac{\sum_{i=1}^m \rho_i s_i}{\sum_{i=1}^m s_i}$

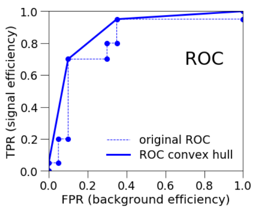
  - Fit the scoring classifier: use ROC* *and* prevalence to determine the local purity $\rho_i = \frac{1}{1+\frac{B_{\text{tot}}}{S_{\text{tot}}}\frac{d\epsilon_b}{d\epsilon_s}}$ in a bin with $s_i = S_{\text{tot}}\, d\epsilon_s$
    - Region of constant ROC slope is a region of constant signal purity

$$\text{FIP2} = \int_0^1 \frac{d\epsilon_s}{1+\frac{1-\pi_s}{\pi_s}\frac{d\epsilon_b}{d\epsilon_s}}$$

Compare FIP2 to AUC: $\text{AUC} = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s$

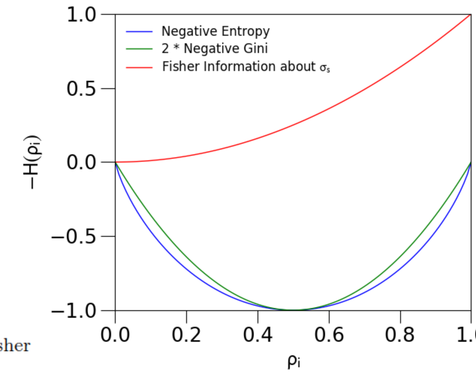


*Technicality (my Python code): convert ROC to *convex hull*
- ensure decreasing slope, i.e. decreasing purity
- avoid staircase effect that would artificially inflate FIP2 (bins of 100% purity: only signal or only background)



FIP2 for training decision trees

- Decision Tree → partition training set *into nodes of different* ρ_i
  - The best split $(n,s)=(n_L,s_L)+(n_R,s_R)$ maximizes $\Delta = -n_L H(\rho_L) - n_R H(\rho_R) + nH(\rho)$
- Current metrics are Gini and entropy: add Fisher information!
  - negative Gini impurity → $-n_i H(\rho_i) = n_i \times [-2\rho_i(1-\rho_i)]$
  - Shannon information → $-n_i H(\rho_i) = n_i \times [\rho_i \log_2 \rho_i + (1-\rho_i)\log_2(1-\rho_i)]$
  - Fisher information on σ_s → $-n_i H(\rho_i) = n_i \times [\rho_i^2]$



- Functions look different, but (modulo a constant factor)…
  - … information gain is the same for Fisher and Gini!

$$\Delta_{\mathrm{Fisher}} = \frac{s_L^2}{n_L} + \frac{s_R^2}{n_R} - \frac{(s_L+s_R)^2}{n_L+n_R} = \frac{(s_L n_R - s_R n_L)^2}{n_L n_R (n_L+n_R)}$$

$$\frac{\Delta_{\mathrm{Gini}}}{2} = -s_L\left(1-\frac{s_L}{n_L}\right) - s_R\left(1-\frac{s_R}{n_R}\right) + (s_L+s_R)\left(1-\frac{s_L+s_R}{n_L+n_R}\right) = \Delta_{\mathrm{Fisher}}$$

- But interpretation is clearer for Fisher: reduce the error on the fit
  - And this is a proof-of-concept for FIP3: split *into nodes of different* $\rho_i \, \frac{1}{s_i}\frac{\partial si}{\partial \theta}$

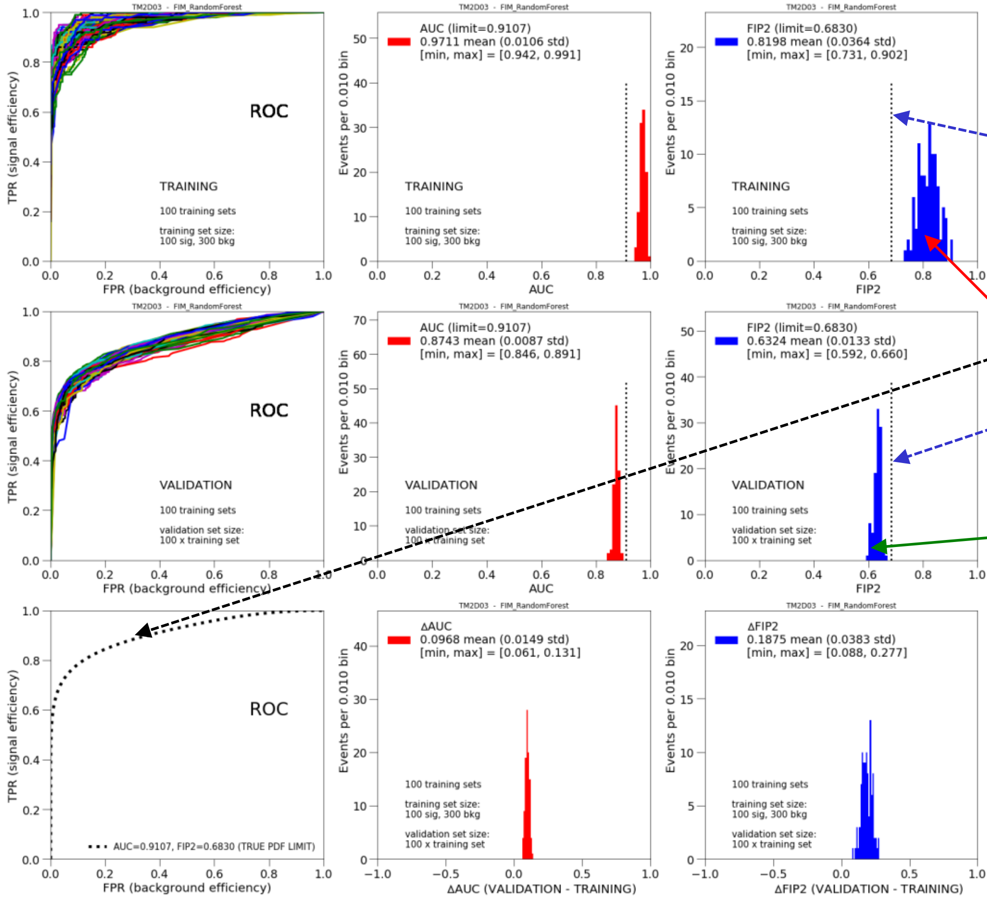
Technicality: user-defined criteria for DecisionTree's will only be available in future sklearn releases
→ I implemented a DecisionTree from scratch, reusing the excellent iCSC notebooks by Thomas Keck (thanks!)

Limits to knowledge

- FIP2 range is [0,1] $\rightarrow$ but it does not mean that 1 is achievable
  - 1 represents the *ideal* case where there is no background
- In some regions of phase space, signal and background events may be undistinguishable based on the available observations
  - There is a limit ROC which depends on the signal and background pdf's
  - There is a limit FIP2 which depends on prevalence and the limit ROC
- Example – toy model, you know the real pdf's and prevalence
  - See next slide about overtraining

Overtraining

- Using the same metric for training and evaluation also simplifies the interpretation of overtraining

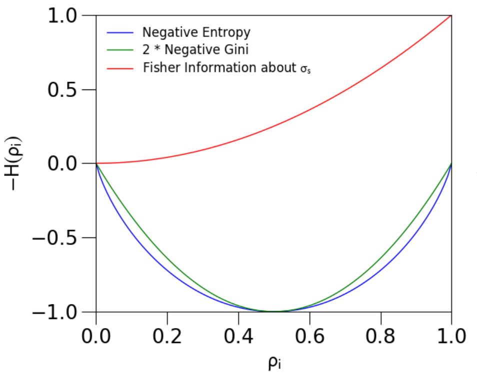


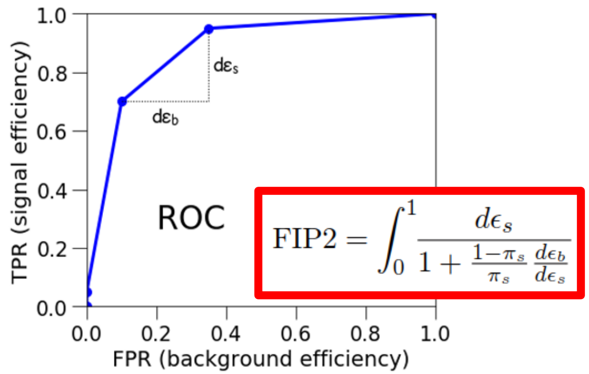
- Example: toy model where you know the real pdf
  - You know the limit ROC
  - You know the limit FIP2
  - You want your validation FIP2 as close as possible to the limit, but it will be lower
  - To get there you maximize your training FIP2, but it will be higher than the real limit
    - You may trace back every increase to one node split
  - You may study the effects of things like min_sample_leaf

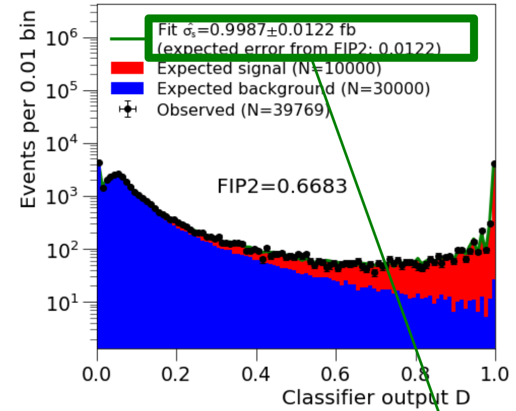
[FIP3] parameter fits including the scoring classifier distribution – *work in progress*

- FIP2 for σ_s fits: one metric for training, evaluation, physics
  - FIP3: one metric for training, evaluation, physics in fits of a generic θ
- Difference with FIP2: include event-by-event sensitivities $\frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$
  - [FIP2] Fit for $\sigma_s \rightarrow$ should partition events into bins of different ρ_i
  - [FIP3] Fit for θ $\rightarrow$ should partition events into bins of different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$
    - Example: a 1-D fit on $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$ or (better) a 2-D fit on ρ_i and $\frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$
- Challenge: what is the value of $\frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$ for real data events?
  - On MC events you can get it from event-by-event MC weight derivatives
  - On data, train a regression tree for $\frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$ on signal only and a decision tree for ρ_i on signal+bkg: use Fisher Information as splitting criterion in both
- *The boundary between classification and regression is blurred!*

Conclusions: one metric to bind them all







TRAINING
- **Fisher Information**
  = measurement error

EVALUATION
- **Fisher Information**
  = measurement error

PHYSICS
- **Fisher Information**
  = measurement error

- One metric for training, evaluation, physics: Fisher Information
- FI meets HEP specificities for evaluation: focuses on signal; describes distribution fits; describes event-by-event sensitivity
  – Different problems need different metrics: HEP needs its own metrics
- The boundary between binary classification and regression is blurred: should partition events into bins of different $\rho_i \frac{1}{s_i}\frac{\partial s_i}{\partial \theta}$

Additional backup slides

Selected slides from my previous IML talks

in April (https://indico.cern.ch/event/668017/contributions/2947015)

and January (https://indico.cern.ch/event/679765/contributions/2814562)

FIP2 from the ROC (+prevalence) or from the PRC

FIP2: integrals on ROC and PRC,
more relevant to HEP than AUC or AUCPR!
(well-defined meaning for distribution fits)

- From the previous slide: $\mathrm{FIP2} = \frac{\sum_{i=1}^{m} \rho_i s_i}{\sum_{i=1}^{m} s_i}$

- FIP2 from the ROC (+prevalence $\pi_s = \frac{S_{\mathrm{tot}}}{S_{\mathrm{tot}} + B_{\mathrm{tot}}}$):

$$S_{\mathrm{sel}} = S_{\mathrm{tot}}\,\epsilon_s, \quad B_{\mathrm{sel}} = B_{\mathrm{tot}}\,\epsilon_b \;\Rightarrow\; s_i = dS_{\mathrm{sel}} = S_{\mathrm{tot}}\,d\epsilon_s, \quad b_i = dB_{\mathrm{sel}} = B_{\mathrm{tot}}\,d\epsilon_b \;\Rightarrow\; \rho_i = \frac{1}{1 + \frac{B_{\mathrm{tot}}}{S_{\mathrm{tot}}}\frac{d\epsilon_b}{d\epsilon_s}} \;\Rightarrow\; \mathrm{FIP2} = \int_0^1 \frac{d\epsilon_s}{1 + \frac{1-\pi_s}{\pi_s}\frac{d\epsilon_b}{d\epsilon_s}}$$

Compare FIP2(ROC) to AUC

$$\mathrm{AUC} = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s$$

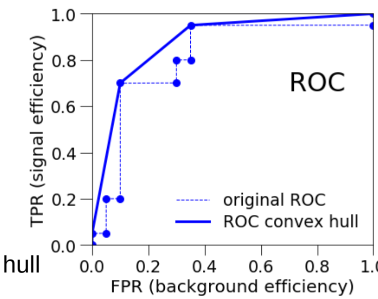
- FIP2 from the PRC:

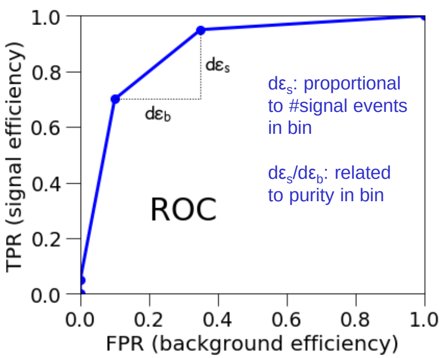
$$S_{\mathrm{sel}} = S_{\mathrm{tot}}\,\epsilon_s, \quad B_{\mathrm{sel}} = S_{\mathrm{sel}}\left(\frac{1}{\rho} - 1\right) \;\Rightarrow\; s_i = dS_{\mathrm{sel}} = S_{\mathrm{tot}}\,d\epsilon_s, \quad b_i = dB_{\mathrm{sel}} = S_{\mathrm{tot}}\left[d\epsilon_s\left(\frac{1}{\rho} - 1\right) - \epsilon_s\frac{d\rho}{\rho^2}\right] \;\Rightarrow\; \rho_i = \frac{\rho}{1 - \frac{\epsilon_s}{\rho}\frac{d\rho}{d\epsilon_s}} \;\Rightarrow\; \mathrm{FIP2} = \int_0^1 \frac{\rho\, d\epsilon_s}{1 - \frac{\epsilon_s}{\rho}\frac{d\rho}{d\epsilon_s}}$$

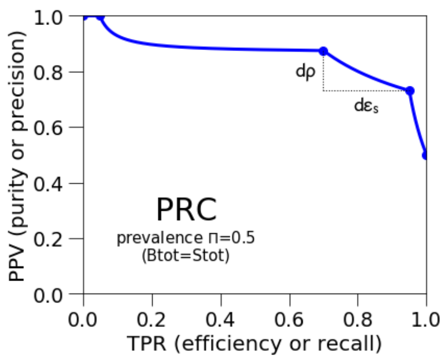
Compare FIP2(PRC) to AUCPR

$$\mathrm{AUCPR} = \int_0^1 \rho\, d\epsilon_s$$

- Easier calculation and interpretation from ROC (+prevalence) than from PRC
  - *region of constant ROC slope** *= region of constant signal purity*
  - decreasing ROC slope = decreasing purity
    - technicality (my Python code): convert ROC to convex hull** first

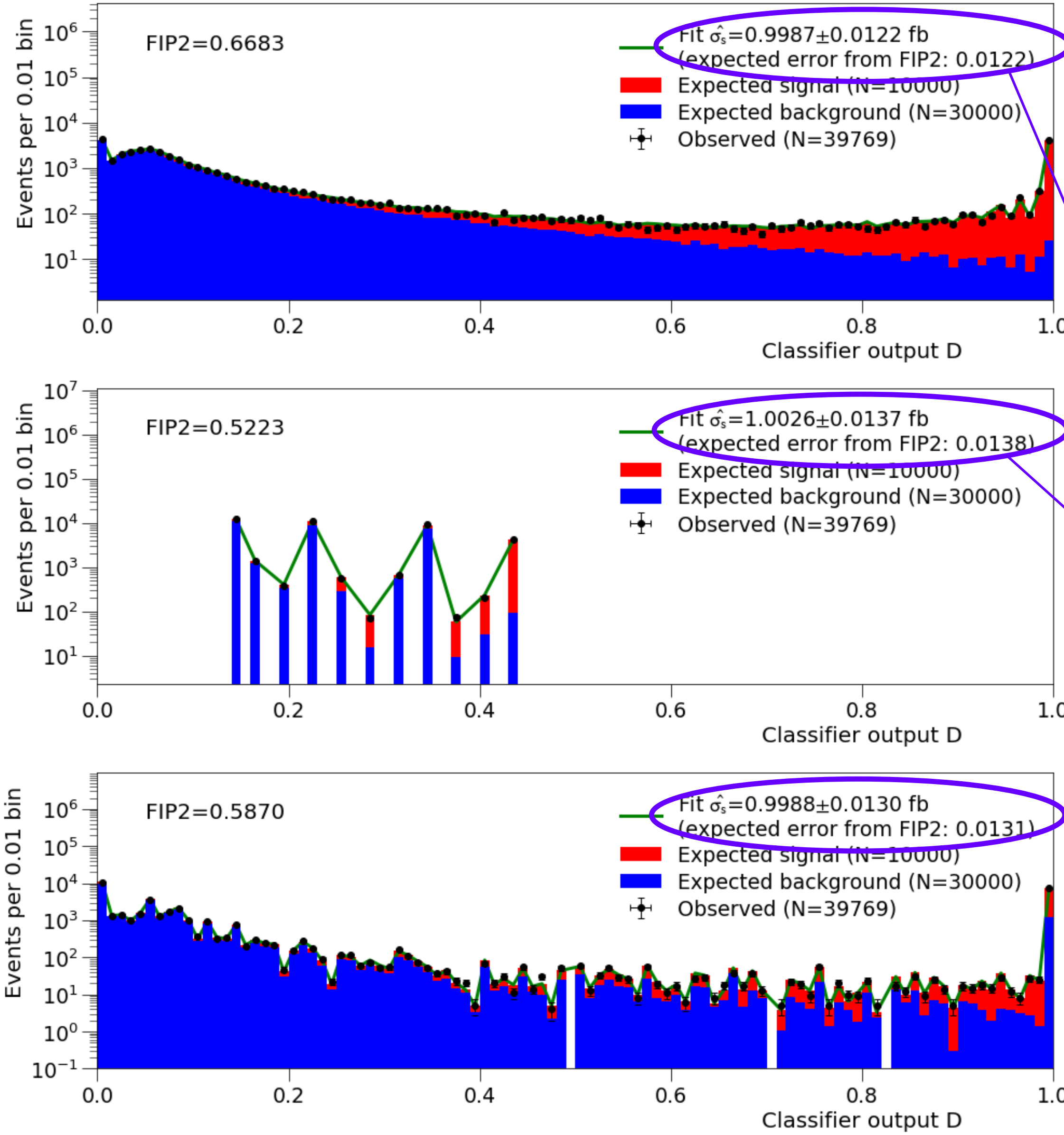






**Convert ROC to convex hull
- ensure decreasing slope
- avoid staircase effect that would artificially inflate FIP2
(bins of 100% purity: only signal or only background)

*ROC slopes are also discussed in medical literature in relation to diagnostic likelihood ratios [Choi 1998], but their use does not seem to be widespread(?)



Sanity check

- Three random forests (on the same 2-D pdf)
  - reasonable
  - undertrained
  - overtrained
- Fit σ_s from the distribution of the classifier output
  - Errors consistent with FIP2

$$(\Delta\hat{\theta}^{(\text{real classifier})})^2 = \frac{1}{\text{FIP}}(\Delta\hat{\theta}^{(\text{ideal classifier})})^2$$

My development environment: SciPy ecosystem, iminuit and bits of rootpy, on SWAN at CERN. Thanks to all involved in these projects!

M by 1D fit to m – visual interpretation

- Information after cuts: $\sum_i \frac{1}{s_i}\left(\frac{\partial si}{\partial M}\right)^2 * \varepsilon_i * \rho_i \rightarrow$ show the 3 terms in each bin i
  - fit = combine N different measurements in N bins $\rightarrow$ local $\varepsilon_{i,}$ ρ_i relevant!
  - important thing is: maximise purity, efficiency in bins with highest sensitivity!

Ideal case - yellow histogram (after cuts) coincides with and covers red histogram (ideal)

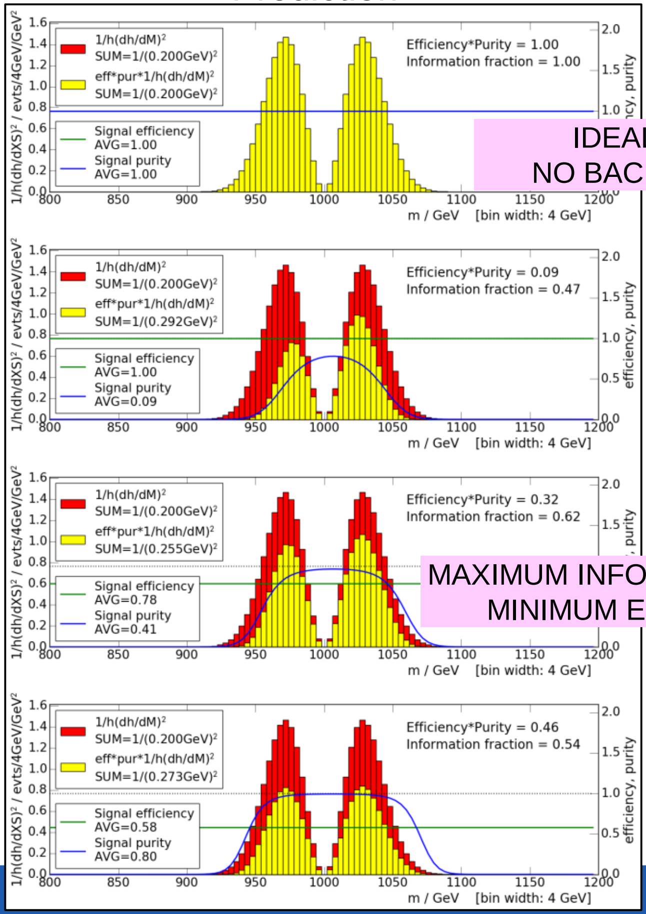
Red histogram: information per bin, ideal case $\frac{1}{s_i}\left(\frac{\partial si}{\partial M}\right)^2$

Blue line: local purity in the bin, ρ_i

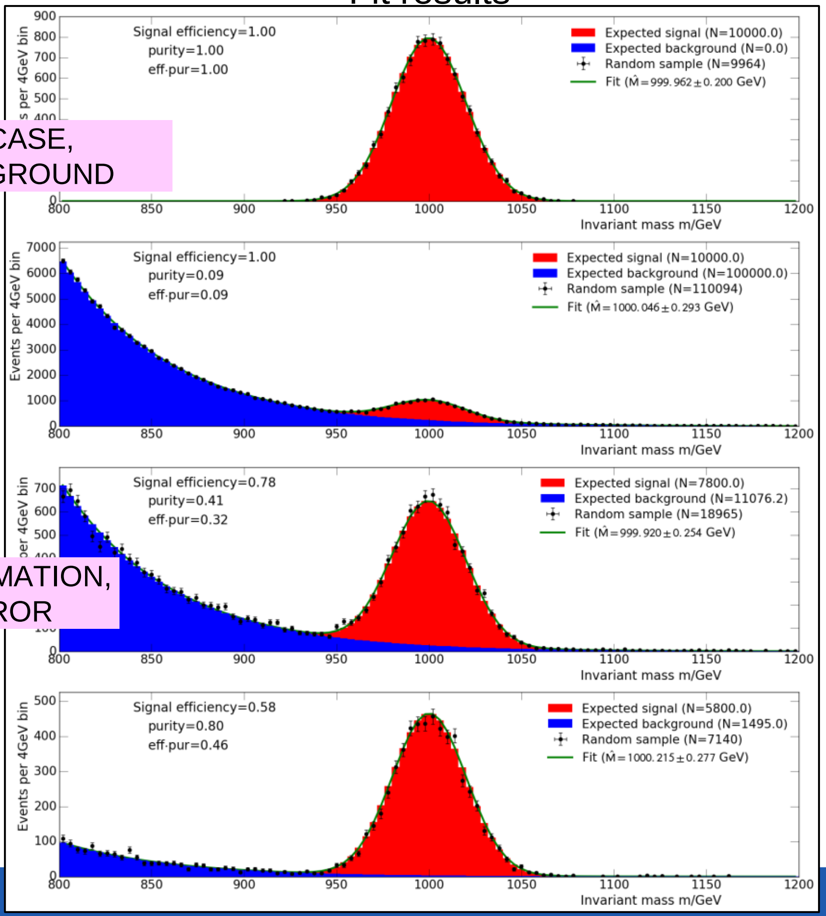
Green line: local efficiency in the bin, ε_i

Yellow histogram: information per bin, after cuts $\varepsilon_i * \rho_i * \frac{1}{s_i}\left(\frac{\partial si}{\partial M}\right)^2$

Prediction



Fit results



IDEAL CASE,
NO BACKGROUND

MAXIMUM INFORMATION,
MINIMUM ERROR

Event selection in HEP searches

- Statistical error in searches by counting experiment → "significance"
  - several metrics → but optimization always involves ϵ_s, ρ alone → TN irrelevant

C. Adam-Bourdarios et al., *The Higgs Machine Learning Challenge*, Proc. NIPS 2014 Workshop on High-Energy Physics and Machine Learning (HEPML2014), Montreal, Canada, PMLR 42 (2015) 19. http://proceedings.mlr.press/v42/cowa14.html

$$Z_0 = \frac{S_\mathrm{sel}}{\sqrt{S_\mathrm{sel}+B_\mathrm{sel}}} \Longrightarrow (Z_0)^2 = S_\mathrm{tot}\epsilon_s\rho$$

Z_0 – Not recommended? (confuses search with measuring σ_s once signal established)

Z_2 – Most appropriate? (also used as "AMS2" in Higgs ML challenge)

$$Z_2 = \sqrt{2\left((S_\mathrm{sel}+B_\mathrm{sel})\log(1+\frac{S_\mathrm{sel}}{B_\mathrm{sel}}) - S_\mathrm{sel}\right)} \Longrightarrow (Z_2)^2 = 2S_\mathrm{tot}\epsilon_s\left(\frac{1}{\rho}\log(\frac{1}{1-\rho})-1\right) = S_\mathrm{tot}\epsilon_s\rho\left(1+\frac{2}{3}\rho+\mathcal{O}(\rho^2)\right)$$

$$Z_3 = \frac{S_\mathrm{sel}}{\sqrt{B_\mathrm{sel}}} \Longrightarrow (Z_3)^2 = S_\mathrm{tot}\epsilon_s\frac{\rho}{1-\rho} = S_\mathrm{tot}\epsilon_s\rho\left(1+\rho+\mathcal{O}(\rho^2)\right)$$

Z_3 ("AMS3" in Higgs ML) – Most widely used, but strictly valid only as an approximation of Z_2 as an expansion in $S_{sel}/B_{sel} \ll 1$?

$$\frac{S_\mathrm{sel}}{B_\mathrm{sel}} = \frac{\rho}{1-\rho} = \rho\left(1+\rho+\mathcal{O}(\rho^2)\right)$$

Expansion in $\rho \ll 1$? – use the expression for Z_2 if anything

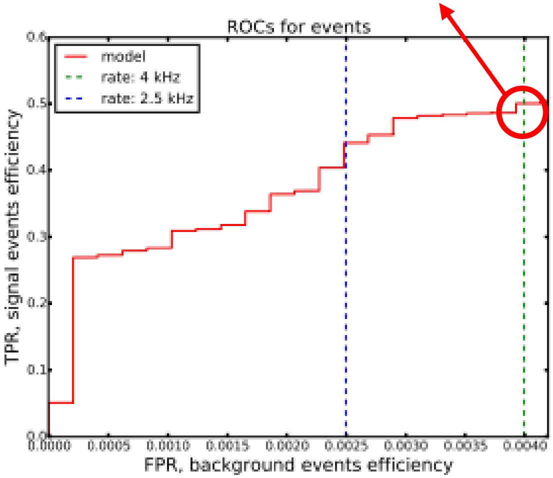
G. Punzi, *Sensitivity of searches for new signals and its optimization*, Proc. PhyStat2003, Stanford, USA (2003). arXiv:physics/0308063v2 [physics.data-an]
G. Cowan, E. Gross, *Discovery significance with statistical uncertainty in the background estimate*, ATLAS Statistics Forum (2008, unpublished). http://www.pp.rhul.ac.uk/~cowan/stat/notes/SigCalcNote.pdf (accessed 15 January 2018)

R. D. Cousins, J. T. Linnemann, J. Tucker, *Evaluation of three methods for calculating statistical significance when incorporating a systematic uncertainty into a test of the background-only hypothesis for a Poisson process*, Nucl. Instr. Meth. Phys. Res. A 595 (2008) 480. doi:10.1016/j.nima.2008.07.086
G. Cowan, K. Cranmer, E. Gross, O. Vitells, *Asymptotic formulae for likelihood-based tests of new physics*, Eur. Phys. J. C 71 (2011) 15. doi:10.1140/epjc/s10052-011-1554-0

- Several other interesting open questions → *beyond the scope of this talk*
  - optimization of systematics? → e.g. see AMS1 in Higgs ML challenge
  - predict significance in a binned fit? → integral over Z^2 (=sum of log likelihoods)?

Trigger

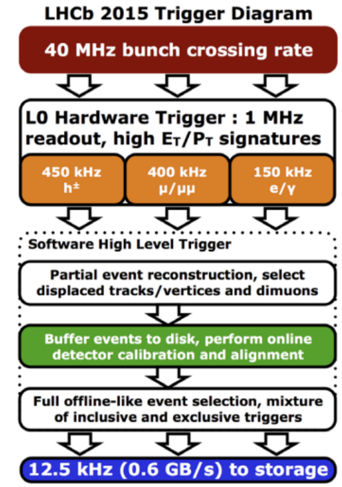
Maximise ε_s at 4 kHz



T. Likhomanenko et al., *LHCb Topological Trigger Reoptimization*, Proc. CHEP 2015, J. Phys. Conf. Series 664 (2015) 082025. doi:10.1088/1742-6596/664/8/082025

Figure 2. Trigger events ROC curve. An output rate of 2.5 kHz corresponds to an FPR of 0.25%, 4 kHz — 0.4%. Thus to find the signal efficiency for a 2.5 kHz output rate, we take 0.25% background efficiency and find the point on the ROC curve that corresponds to this FPR.

IIUC, 4kHz is ε_b (FPR) = 0.4% of 1 MHz L0 hw rate

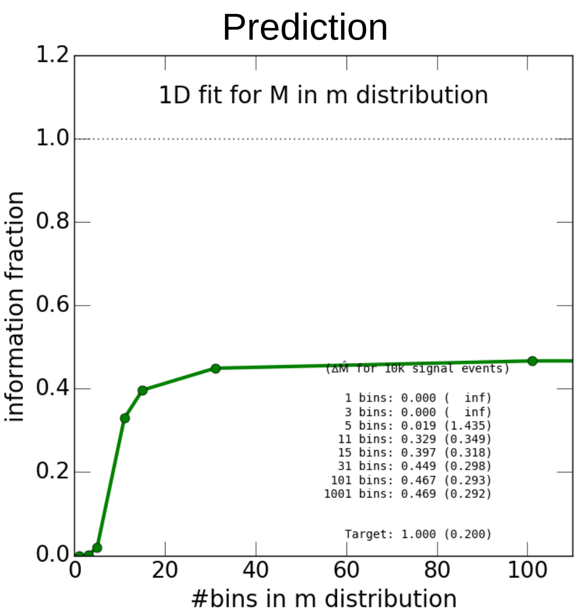


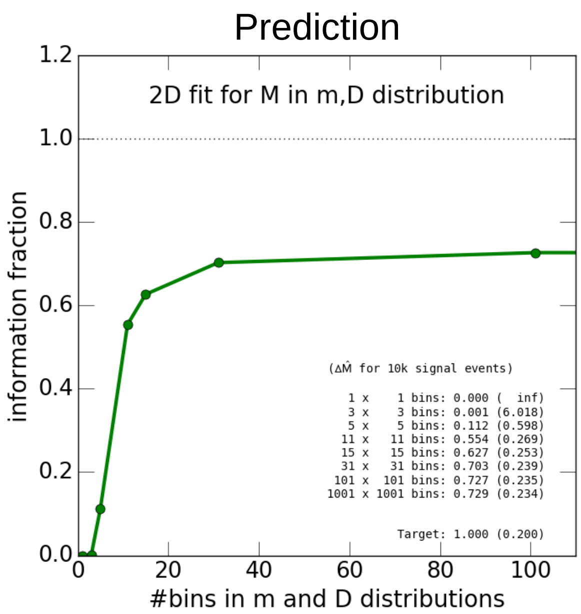
F. Dordei, *LHCb detector and trigger performance in Run II*, Proc. 5th Int. Conf. on New Frontiers in Physics (ICNFP 2016), EPJ Web of Conferences 164, 01016 (2017). doi:10.1051/epjconf/201716401016

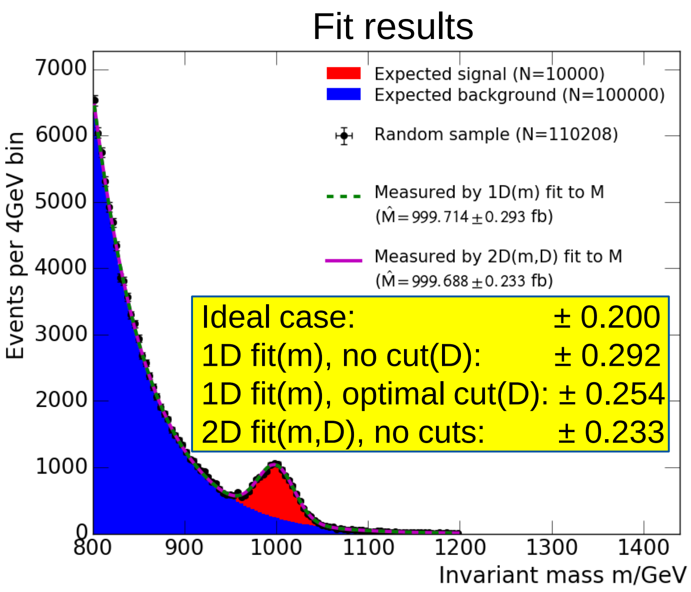
- Different meaning of absolute numbers in the confusion matrix
  - Trigger → events per unit time i.e. trigger rates
  - (Physics analyses → total event sample sizes i.e. total integrated luminosities)
- Binary classifier optimisation goal: maximise ε_s for a given B_{sel} per unit time
  - i.e. maximise TP/(TP+FN) for a given FP → TN irrelevant
- Relevant plot → ε_s vs. B_{sel} per unit time (i.e. *TPR vs FP*)
  - ROC curve (*TPR vs. FPR*) confusing – ***AUC irrelevant***
  - e.g. maximise ε_s for 4 kHz trigger rate, whether L0 rate is 1 MHz or 2MHz

M by 2D fit – use classifier to partition, not to cut

- Showed a fit for M on m, after a cut on D $\rightarrow$ can also fit in 2-D with no cuts
  - again, use the scoring classifier D to partition data, not to reject events
- Why is binning so important, especially using a discriminating variable?
  - next slide...







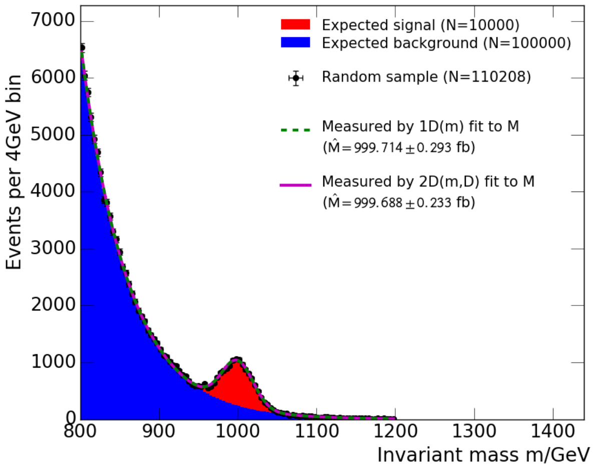
Optimal partitioning – optimal variables

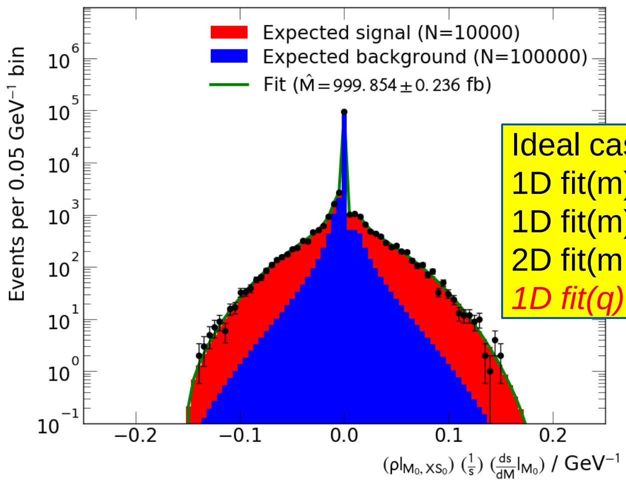
- The previous slide implies that q = $\rho \frac{1}{s}\frac{\partial s}{\partial \theta}$ is an optimal variable to fit for θ
  - proof of concept → 1-D fit of q has the same precision on M as 2-D fit of (m,D)
  - closely related to the "optimal observables" technique

M. Davier, L. Duflot, F. LeDiberder, A. Rougé, *The optimal method for the measurement of tau polarization*, Phys. Lett. B 306 (1993) 411. doi:10.1016/0370-2693(93)90101-M

M. Diel, O. Nachtmann, *Optimal observables for the measurement of three-gauge-boson couplings in $e^+e^- \to W^+W^-$*, Z. Phys. C 62 (1994) 397. doi:10.1007/BF01555899

O. Nachtmann, F. Nagel, *Optimal observables and phase-space ambiguities*, Eur. Phys. J. C40 (2005) 497. doi:10.1140/epjc/s2005-02153-9





Ideal case:	± 0.200
1D fit(m), no cut(D):	± 0.292
1D fit(m), optimal cut(D):	± 0.254
2D fit(m,D), no cuts:	± 0.233
1D fit(q):	*± 0.236*

- In practice: train one ML variable to reproduce $\frac{1}{s}\frac{\partial s}{\partial \theta}$?
  - not needed for cross-sections or searches (this is constant)