

Optimising HEP parameter fits: event-by-event sensitivities, weight derivative regression

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This is a follow-up of my CHEP2018 talk about binned fits of a parameter θ

Evaluation and training metrics: Fisher Information Part

Previous CHEP2018 talk

Event selection
Binary classification

Bin-by-bin sensitivity to θ

Cross-section fits (FIP1, FIP2)

Medical Diagnostics (AUC), Information Retrieval (F1)

Talk: https://doi.org/10.5281/zenodo.1303387
Paper: https://doi.org/10.1051/epiconf/201921406004

This CHEP2019 talk

Event partitioning Non-binary regression

WEIGHT DERIVATIVE REGRESSION

Event-by-event sensitivity to θ

MINIMUM ERROR WITH AN IDEAL DETECTOR

Mass fits, Coupling fits (FIP3)

Meteorology (MSE, Brier), Medical Prognostics

Compare to and learn from other domains

Outline

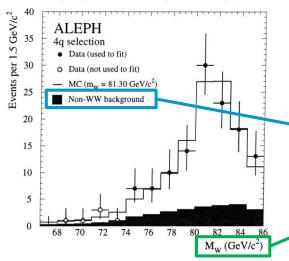
- 1 HEP parameter fits and Weight Derivative Regression
- 2 Learning from others
- Conclusions

This talk only provides some maths and some literature review

No toy model or concrete applications are presented



ALEPH Collaboration, Measurement of the W mass by direct reconstruction in e^+e^- collisions at 172 GeV, Phys. Lett. B 422 (1998) 384. doi:10.1016/S0370-2693(98)00062-8



There are two handles to minimize the statistical error $\Delta\theta$:

1. Event selection

Signal-background discrimination

2. Event partitioning Variable(s) for the distribution fit

My CHEP2018 talk: event selection

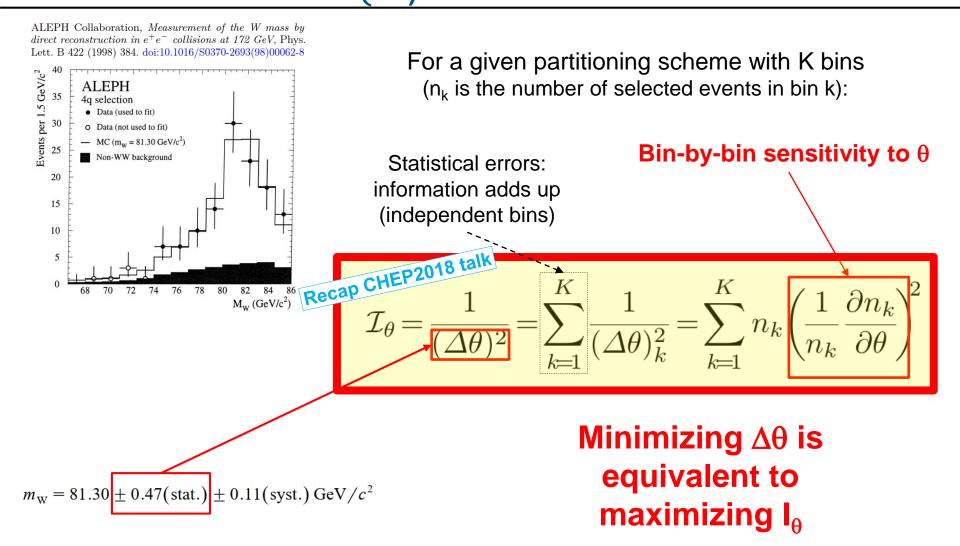
This CHEP2019 talk: event partitioning (selection is a special case of partitioning)

$$m_{\rm W} = 81.30 \pm 0.47 ({\rm stat.}) \pm 0.11 ({\rm syst.}) \,{\rm GeV}/c^2$$

I only discuss the statistical error Δθ in this talk

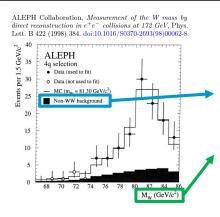
(I ignore systematic errors, even if at LHC they are the limitation)

Fisher Information $\frac{1}{(\Delta\theta)^2}$ from bin-by-bin sensitivities





Fisher Information Part (FIP)



There are two handles to minimize the statistical error $\Delta\theta$:

- 1. Event selection Signal-background discrimination
- 2. Event partitioning Variable(s) for the distribution fit

My CHEP2018 talk: FIP evaluation of event selection

For a given data set and given partitioning, FIP compares I₀ to I₀ (ideal) for the ideal selection (select all signal, reject all bkg)

Recap CHEP2018 talk FIP evaluation of event partitioning

For a given data set, FIP compares I_{θ} to $I_{\theta}^{(ideal)}$ for the ideal partitioning (and the ideal selection)

This CHEP2019 talk:

But what is the smallest statistical error achievable on a given data set with ideal partitioning and selection? Enter event-by-event sensitivities

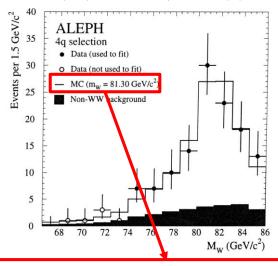
Fisher Information Part (FIP): the fraction of the information available "in an ideal case" retained by a given analysis

$$FIP = \frac{\mathcal{I}_{\theta}}{\mathcal{I}_{\theta}^{(ideal)}} = \frac{(\Delta \theta^{(ideal)})^2}{(\Delta \theta)^2} \le 100\%$$

FIP is a metric between 0 and 1 – higher is better

Event-by-event Monte Carlo reweighting

ALEPH Collaboration, Measurement of the W mass by direct reconstruction in e^+e^- collisions at 172 GeV, Phys. Lett. B 422 (1998) 384. doi:10.1016/S0370-2693(98)00062-8



$$w_{i}(m_{\mathrm{W}}, \Gamma_{\mathrm{W}}) = \frac{|\mathcal{M}(m_{\mathrm{W}}, \Gamma_{\mathrm{W}}, p_{i}^{1}, p_{i}^{2}, p_{i}^{3}, p_{i}^{4})|^{2}}{|\mathcal{M}(m_{\mathrm{W}}^{\mathrm{MC}}, \Gamma_{\mathrm{W}}^{\mathrm{MC}}, p_{i}^{1}, p_{i}^{2}, p_{i}^{3}, p_{i}^{4})|^{2}}$$

Fit for $\theta \rightarrow$ Compare data in bin k to

model prediction n_k as a function of θ

$$n_k(\theta) = \sum_{i \in k} w_i(\theta) = \sum_{i \in k}^{\text{Sig}} w_i(\theta) + \sum_{i \in k}^{\text{Bkg}} w_i = s_k(\theta) + b_k$$

- 1. Generate signal sample at θ_{ref} , with $w_i(\theta_{ref})=1$ (By definition, background does not depend on θ)
- 2. Full detector simulation
 (MC truth event properties x_i(true) → observed event properties x_i)
- 3. Reweight each event by matrix element ratio

$$w_i(\theta) = \frac{\text{Prob}_{(\theta)}(\mathbf{x}_i^{(\text{true})})}{\text{Prob}_{(\theta_{\text{ref}})}(\mathbf{x}_i^{(\text{true})})} = \frac{|\mathcal{M}(\theta, \mathbf{x}_i^{(\text{true})})|^2}{|\mathcal{M}(\theta_{\text{ref}}, \mathbf{x}_i^{(\text{true})})|^2}$$

Monte Carlo reweighting: used extensively at LEP Simpler than Matrix Element Method (no integration) [see Gainer2014, Mattelaer2016 for hadron colliders]

J. S. Gainer, J. Lykken, K. T. Matchev, S. Mrenna, M. Park, Exploring theory space with Monte Carlo reweighting, JHEP 2014 (2014) 78. doi:10.1007/JHEP10(2014)078

O. Mattelaer, On the maximal use of Monte Carlo samples: re-weighting events at NLO accuracy, Eur. Phys. J. C 76 (2016) 674. doi:10.1140/epjc/s10052-016-4533-7



Event-by-event sensitivities γ_i : MC weight derivatives

Bin-by-bin model prediction $n_k(\theta)$

$$n_k(\theta) = \sum_{i \in k} w_i(\theta) = \sum_{i \in k}^{\text{Sig}} w_i(\theta) + \sum_{i \in k}^{\text{Bkg}} w_i = s_k(\theta) + b_k$$

Define the **event-by-event sensitivity** γ_i **to** θ as the *derivative with respect to* θ *of the MC weight* w_i

$$\gamma_i|_{\theta} = \left(\frac{1}{w_i}\frac{\partial w_i}{\partial \theta}\right)_{\theta} \longrightarrow \gamma_i = \gamma_i|_{\theta=\theta_{\text{ref}}} = \left(\frac{\partial w_i}{\partial \theta}\right)_{\theta=\theta_{\text{ref}}}$$

(normalized by $1/w_i$, but $w_i(\theta_{ref})=1$ at the reference $\theta=\theta_{ref}$)

The bin-by-bin sensitivity to θ in bin k is the average in bin k of the event-by-event sensitivity γ_i to θ

$$\left(\frac{1}{n_k} \frac{\partial n_k}{\partial \theta}\right)_{\theta = \theta_{\text{ref}}} = \frac{1}{n_k} \sum_{i \in k} \gamma_i = \langle \gamma \rangle_k = \frac{1}{n_k} \frac{\partial n_k}{\partial \theta}$$

Beyond the signal-background dichotomy

Background events have $\gamma_i=0$

because by definition they are insensitive to θ

$$\gamma_i = \left(\frac{1}{w_i} \frac{\partial w_i}{\partial \theta}\right) = 0,$$
 if $i \in \{\text{Background}\}$

$$\gamma_i = \left(\frac{1}{w_i} \frac{\partial w_i}{\partial \theta}\right) \in \{-\infty, +\infty\}, \quad \text{if } i \in \{\text{Signal}\}$$

Signal events may have sensitivity $\gamma_i > 0$, $\gamma_i = 0$ or $\gamma_i < 0$ (special case: cross-section fit $\gamma_i=1/\sigma_s$)

For what concerns statistical errors in a parameter fit, there is no distinction between background events and signal events with low sensitivity ($|\gamma_i| \sim 0$)

 $\phi_k = \langle \gamma \rangle_{k, \text{Sig}} = \frac{1}{s_k} \sum_{i=1}^{(\text{Sig})} \gamma_i = \frac{1}{s_k} \frac{\partial s_k}{\partial \theta}$ Bin-by-bin sensitivity ϕ_k of signal events alone:

Bin-by-bin sensitivity $\langle \gamma \rangle_k$ $\langle \gamma \rangle_k = \frac{1}{n_k} \frac{\partial n_k}{\partial \theta} = \frac{\rho_k}{s_k} \frac{\partial s_k}{\partial \theta} = \rho_k \phi_k$ of signal + background:

Effect of background: it dilutes by a factor $\rho_k \leq 1$ the bin-by-bin sensitivity and information for signal events alone

Information from all bins for signal + background:

$$\mathcal{I}_{\theta} = \sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2 = \sum_{k=1}^{K} n_k (\rho_k \phi_k)^2 = \sum_{k=1}^{K} s_k \rho_k \phi_k^2$$

Ideal case: partition by the evt-by-evt sensitivity γ_i

Information I_{θ} in terms of average bin-by-bin sensitivities:

$$\mathcal{I}_{\theta} = \sum_{k=1}^{K} n_k \left(\frac{1}{n_k} \frac{\partial n_k}{\partial \theta} \right)^2 = \sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2$$

There is an information gain in partitioning two events i_1 and i_2 in two 1-event bins rather than one 2-event bin if their sensitivities γ_{i_1} and γ_{i_2} are different

$$\Delta \mathcal{I}_{\theta} = \gamma_{i_1}^2 + \gamma_{i_2}^2 - 2\left(\frac{\gamma_{i_1} + \gamma_{i_2}}{2}\right)^2 = \frac{1}{2}(\gamma_{i_1} - \gamma_{i_2})^2$$



Goal of a distribution fit: partition events by their different MC-truth event-by-event sensitivities γ_i to θ



How to achieve this in practice: next two slides (WDR)

Use $I_{\theta}^{(ideal)}$ to compute FIP: following two slides



Knowing one's limits: maximum achievable information with an ideal detector

- Ideal acceptance, select all signal events S_{sel}=S_{tot}
- Ideal resolution, measured γ_i is that from MC truth (implies ideal rejection of background events, γ_i =0)

$$\mathcal{I}_{\theta}^{(\text{ideal})} = \sum_{i=1}^{N_{\text{tot}}} \gamma_i^2 = \sum_{i=1}^{S_{\text{tot}}} \gamma_i^2$$

Weight Derivative Regression (WDR): train q_i for γ_i

Goal of a distribution fit: separate events with different MC-truth event-by-event sensitivities γ_i to θ

But γ_i is not observable on real data events!

Weight Derivative Regression:

train a regressor $q_i = q(x_i)$ on detector-level MC observables $x_i \implies$ against the MC-truth $\gamma_i = \partial w_i/\partial \theta$ for signal and background MC events

Then determine θ
 ⇒ by the 1-D fit of q(x_i)
 for real data events x_i

Some of many caveats:

- Dependency of weight derivative on reference θ_{ref} : WDR easier for coupling fits than for mass fits?
- How feasible is it to compute and store MC-truth weight derivatives?
- How useful is this for measurements limited by systematics?
- Train q on signal + background and 1-D fit of q, or train q on signal alone and 2-D fit on q and scoring classifier?
- How to deal with simultaneous fits of many parameters?

Training metric: maximize FIP Evaluation metric: maximize FIP

(or equivalently minimize MSE? see final slides)



WDR and **Optimal Observables**

The WDR idea was inspired by the Optimal Observables (OO) method

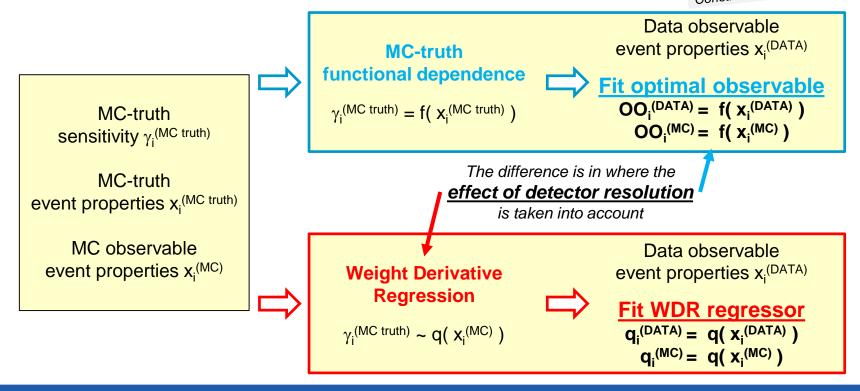
Both OO and WDR partition data by an approximation of a MC-truth sensitivity γ_i to θ (OO does not use MC weight derivatives but it is similar)

D. Atwood, A. Soni, Analysis for magnetic moment and electric dipole moment form factors of the top quark via $e^+e^- \rightarrow t\bar{t}$, Phys. Rev. D 45 (1992) 2405. doi:10.1103/PhysRevD.45.2405,

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)9010 M M. Diehl, O. Nachtmann, Optimal observables for the measurement of three-gauge-boson couplings in $e^+e^- \rightarrow W^+W^-$, 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

Like OO, WDR can be useful in coupling/EFT fits (more than in mass fits)

Some similarities also with the MadMiner approach
See CHEP 2019 contribution #506
"Constraining effective field theories with ML"



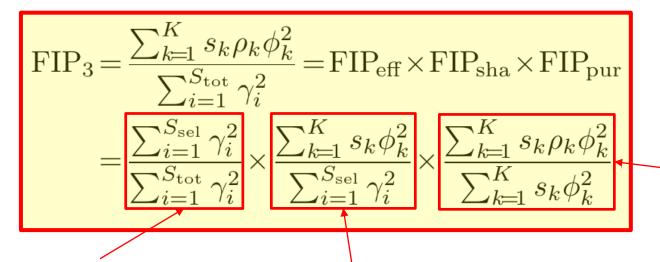


FIP decomposition: efficiency, sharpness, purity

Numerator: Information retained by a given analysis using $N_{sel} = \sum n_k$ events with the given detector

Denominator: maximum theoretically available information from the given sample of N_{tot} events (S_{tot} signal events) if the true γ_i were known for each event (ideal detector)

$$FIP_3 = \frac{\mathcal{I}_{\theta}}{\mathcal{I}_{\theta}^{(ideal)}} = \frac{\sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2} = \frac{\sum_{k=1}^{K} s_k \rho_k \phi_k^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2}$$



Sensitivity-weighted signal efficiency:

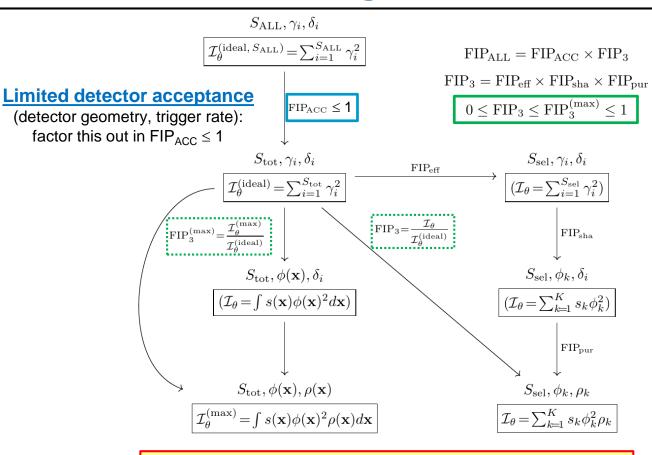
keep S_{sel} of S_{tot} events

Sharpness

in separating signal events with different sensitivities: partition S_{sel} signal events into K bins

"sharpness" as in meteorology: see later why Sensitivity-weighted
signal purity
or equivalently
sharpness in separating
signal events
from background events:
dilution of signal sensitivity
caused by bin-by-bin purity ρ_k

Limits to knowledge: FIP for a realistic detector



Limited detector resolution

In the multi-dimensional space of event observables **x**, it is impossible to resolve:

signal events
 with high sensitivity γ_i
 from signal events
 with low sensitivity γ_i:
 average sensitivity is φ(x)

- signal events δ_i =1 from background events δ_i =0: average purity is $\rho(\mathbf{x})$

FIP is a metric in [0,1], but the detector acceptance and resolution limit it to $0 \le FIP \le FIP^{(max)} < 1$

 $ightharpoonup FIP>FIP^{(max)}$ while training q_i implies **overtraining**...



2 – Learning from others

Reading Room, British Museum
Diliff (own work, unmodified) CC BY 2.5



Different problems in different domains require different metrics and tools...

2 – Learning from others

Evaluating the evaluation metrics

Evaluation metrics of (binary and non-binary) classifiers have been analysed and compared in many ways

There are two approaches which I find particularly useful:

1. Studying the symmetries and invariances of evaluation metrics

M. Sokolova, G. Lapalme, A Systematic Analysis of Performance Measures for Classification Tasks, Information Processing and Management 45 (2009) 427. doi:10.1016/j.ipm.2009.03.002 A. Luque, A Carrasco, A. Martin, J. R. Lama, Exploring Symmetry of Binary Classification Performance Metrics, Symmetry 11 (2019) 47. doi:10.3390/sym11010047.

Example: (ir)relevance of True Negatives: in my CHEP2018 talk

2. Separating threshold, ranking and probabilistic metrics

R. Caruana, A. Niculescu-Mizil, Data mining in metric space: an empirical analysis of supervised learning performance criteria, Proc. 10th Int. Conf. on Knowledge Discovery and Data Mining (KDD-04), Seattle (2004). doi:10.1145/1014052.1014063

Example: AUC (ranking) vs. MSE (probabilistic): in this CHEP2019 talk (next 3 slides)

- C. Ferri, J. Hernández-Orallo, R. Modroiu, An Experimental Comparison of Classification Performance Metrics, Proc. Learning 2004, Elche (2004). http://dmip.webs.upv.es/papers/Learning2004.pdf
- C. Ferri, J. Hernández-Orallo, R. Modroiu, An Experimental Comparison of Performance Measures for Classification, Pattern Recognition Letters 30 (2009) 27. doi:10.1016/j.patrec.2008.08.010



2 – Learning from others: Meteorology

MSE decomposition: Validity and Sharpness

MSE (mean squared error) of regressor prediction q_i versus the true γ_i for event i:

$$MSE = \frac{1}{N_{\text{tot}}} \sum_{i=1}^{N_{\text{tot}}} (q_i - \gamma_i)^2$$

MSE is a probabilistic metric for both evaluation and training

MSE decomposition

(if the N_{tot} events are split into K partitions, with $q_i=q_{(k)} \ \forall i \in k$):

Validity, Reliability, Calibration

$$MSE = \frac{1}{N_{\text{tot}}} \left[\sum_{k=1}^{K} n_k (q_{(k)} - \langle \gamma \rangle_k)^2 \right] +$$

Validity: in a partition with given true average sensitivity $<\gamma_k>$, is the predicted sensitivity $q_{(k)}$ well calibrated?

~0 in training by construction ~0 in evaluation if there are no systematics

Paraphrases the "Brier score" decomposition in Meteorology

G. W. Brier, Verification of forecasts expressed in terms of probability, Weather Rev. 78 (1950) 1. doi:10.1175/1520-0493(1950)078%3C0001:VOFEIT%3E2.0.CO;2

F. Sanders, On Subjective Probability Forecasting, J. Applied Meteorology 2 (1963) 191. https://www.jstor.org/stable/26169573

Sharpness, Resolution, Refinement

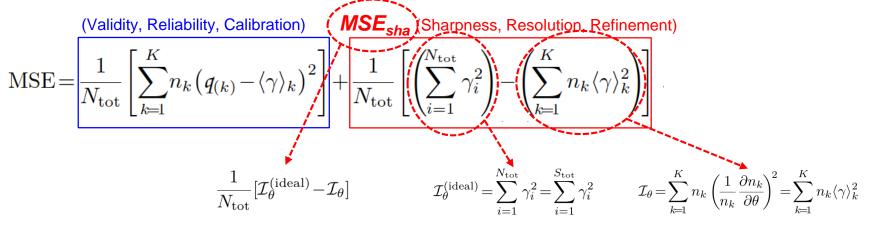
$$\frac{1}{N_{\text{tot}}} \left[\left(\sum_{i=1}^{N_{\text{tot}}} \gamma_i^2 \right) - \left(\sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2 \right) \right]$$

Sharpness: how well do we <u>separate</u> events with different true sensitivities γ_i ?

This is what determines the statistical error on the measurement of θ : related to FIP!

2 – Leaning from others: Meteorology

FIP is related to Sharpness (MSE)



FIP is related to Sharpness:

In the ideal case: $MSE_{sha}=0$ and FIP=1 (events with different γ_i can be resolved)

$$FIP = \frac{\mathcal{I}_{\theta}}{\mathcal{I}_{\theta}^{(ideal)}} = \left(1 - \frac{N_{tot} \times MSE_{sha}}{\mathcal{I}_{\theta}^{(ideal)}}\right)$$

Practical implication for Weight Derivative Regression:

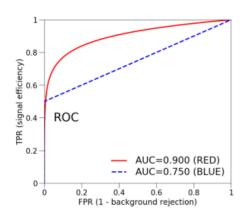
MSE is the most appropriate loss function for training the WDR regressor

2 – Learning from others: HEP does not need ranking, or ranking metrics HEP needs partitioning, and probabilistic metrics

Ranking, and ranking metrics

Pick two events at random and rank them

Medical Diagnostics → <u>ranking</u> evaluation of diagnostic prediction
Patient A is diagnosed as more likely sick than B: how often am I right?



- D. M. Green, General Prediction Relating Yes-No and Forced-Choice Results, J. Acoustical Soc. Am. 36 (1964) 1042. doi:10.1121/1.2143339
- D. J. Goodenough, K. Rossmann, L. B. Lusted, Radiographic applications of signal detection theory, Radiology 105 (1972) 199. doi:10.1148/105.1.199
- J. A. Hanley, B. J. McNeil, The meaning and use of the area under a receiver operating characteristic (RCC) curve, Radiology 143 (1982) 29. doi:10.1148/radiology.143.1.7063747 A. P. Bradley, The use of the area under the RCC curve in the evaluation of Machine Learning algorithms, Pattern Recognition 30 (1997) 1145. doi:10.1016/S0031-3203(96)00142-2

<u>AUC (Area Under the ROC Curve)</u>: probability that a randomly chosen diseased subject is correctly rated or <u>ranked</u> with greater suspicion than a randomly chosen non-diseased subject

IRRELEVANT FOR HEP PARAMETER FITS?

Partitioning, and probabilistic metrics

Group events and make a forecast on each subset

Meteorology → <u>probabilistic</u> evaluation of weather prediction Rain forecast was 30% for these 10 days: actual rainy days?

Medical Prognostics → <u>probabilistic</u> evaluation of survival prediction 5yr survival forecast was 90% for these 10 patients: actual survivors?

HEP parameter fits \rightarrow *probabilistic evaluation of measurement of* θ MC forecast for #events in this bin is 10 (20) for θ =1 (2): actual data?

$$\text{MSE} = \underbrace{\frac{1}{N_{\text{tot}}} \left[\sum_{k=1}^{K} n_k \left(q_{(k)} - \langle \gamma \rangle_k \right)^2 \right]}_{\text{Ntot}} + \underbrace{\frac{1}{N_{\text{tot}}} \left[\left(\sum_{i=1}^{N_{\text{tot}}} \gamma_i^2 \right) - \left(\sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2 \right) \right]}_{\text{Ntot}}$$

Sharpness (from MSE): how well can I resolve days with 10% and 90% chance of rain? Patients with 10% and 90% 5yr survival rate? Signal events with high sensitivity to θ from (signal or background) events with low sensitivity?

ESSENTIAL FOR HEP PARAMETER FITS!

Conclusions – HEP measurement of a parameter θ

- MC weight derivatives (event-by-event sensitivities γ_i to θ) may be used :
 - -To determine the ideal partitioning strategy: partition by γ_i
 - -To derive the minimum error on the measurement of θ (ideal detector)

$$\mathcal{I}_{\theta}^{(\text{ideal})} = \sum_{i=1}^{N_{\text{tot}}} \gamma_i^2 = \sum_{i=1}^{S_{\text{tot}}} \gamma_i^2$$

-To derive training and validation metrics to optimize the measurement

$$\text{FIP} = \frac{\mathcal{I}_{\theta}}{\mathcal{I}_{\theta}^{\text{(ideal)}}} = \frac{\sum_{k=1}^{K} n_k \langle \gamma \rangle_k^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2} = \frac{\sum_{k=1}^{K} s_k \rho_k \phi_k^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2}$$

Evaluation and training metrics: FIP

- -To train a regressor q_i of γ_i (optimal observable) for a 1-D fit of θ
- HEP parameter fits are closer to Meteorology than to Medical Diagnostics
 - -They use partitioning and need probabilistic metrics (sharpness, MSE)

$$FIP = \frac{\mathcal{I}_{\theta}}{\mathcal{I}_{\theta}^{\text{(ideal)}}} = \left(1 - \frac{N_{\text{tot}} \times MSE_{\text{sha}}}{\mathcal{I}_{\theta}^{\text{(ideal)}}}\right)$$

Compare to and learn from other domains

-They do not use ranking and do not need ranking metrics (AUC)

Backup slides

Non-dichotomous truth: examples

- Medical Diagnostics → continuous scale gold standard
 - The Obuchowski measure, e.g. five stages of liver fibrosis,

N. A. Obuchowski, An ROC-Type Measure of Diagnostic Accuracy When the Gold Standard is Continuous-Scale, Statistics in Medicine 25 (2006) 481, doi:10.1002/sim.2228 M. J. Pencina, R. B. D'Agostino, Overall C as a measure of discrimination in survival analysis: model specific population value and confidence interval estimation. Statistics in Medicine 23 (2004) 2109. doi:10.1002/sim.1802

J. Lambert et al., How to Measure the Diagnostic Accuracy of Noninvasive Liver Fibrosis Indices: The Area Under the ROC Curve Revisited, Clinical Chemistry 54 (2008) 1372 doi:10.1373/clinchem.2007.097923

- Information Retrieval → graded relevance assessment and
 - Discounted Cumulated Gain $\operatorname{DCG}[k] = \sum_{i=1}^{k} \frac{\operatorname{G}[i]}{\min(1, \log_2 i)}$

K. Järvelin, J. Kekäläinen, IR evaluation methods for retrieving highly relevant documents, Proc. 23rd ACM SIGIR Conf. (SIGIR 2000), Athens (2000). doi:10.1145/345508.345545 J. Kekäläinen, K. Järvelin, Using graded relevance assessments in IR evaluation, J. Am. Soc. Inf. Sci. 53 (2002) 1120.

K. Järvelin, J. Kekäläinen, Cumulated gain-based evaluation of IR techniques, J. ACM Trans. on Inf. Sys. (TOIS) 20

- **ML** (for finance) → example-dependent cost-sensitive classif
 - fraudulent legitimate – Payoff matrix for transaction x\$: \$20 -\$20Response: yes/no decision 0.02xapprove

costs and probabilities are both unknown, Proc. 7th Int. Conf. on Knowledge Discovery and Data Mining (KDD-01), San Francisco (2001). doi:10.1145/502512.502540 C. Elkan, The Foundations of Cost-Sensitive Learning, Proc.

17th Int. Joint Conf. on Artificial Intelligence (IJCAI-01),

- Meteorology → probabilistic evaluation of weather forecasts
 - Rain forecast was 30% for these 10 days: actual rainy days?

G. W. Brier, Verification of forecasts expressed in terms of probability, Weather Rev. 78 (1950) 1. doi:10.1175/1520-0493(1950)078%3C0001:VOFEIT%3E2.0.CO;2

F. Sanders, On Subjective Probability casting, J. Applied Meteorology 2 (1963) 191 https://www.jstor.org/stable/26169573

Medical Prognostics → probabilistic evaluation of survival forecasts

- 5yr survival forecast was 90% for these 10 patients: actual survivors?
- HEP measurement of $\theta \rightarrow evt$ -by-evt sensitivity to θ

D. J. Spiegelhalter, Probabilistic prediction in patient management and clinical trials, Statist. Med. 5 (1986) 421. doi:10.1002/sim.4780050506

F. E. Harrell, K. L. Lee, D. B. Mark, Multivariable prognostic models: issues in developing models, evaluating assumptions and adequacy, and measuring and reducing errors, Statist. Med. 15 (1996) 361. 10.1002/(SICI)1097-0258(19960229)15:4<361::AID-SIM168>3.0.CO;2-4



Weight Derivative Regression – in practice

- Compute event-by-event sensitivities γ_i from signal MC weight derivatives
 - -Possibly at various reference values of θ
- Pre-select events to remove most backgrounds
 - –Possibly maximizing a sensitivity-weighted signal efficiency?
- Train a regressor q_i for the MC-truth γ_i from measured event properties
 - -Possibly using MSE as the loss function in the training (see next slides)
- Determine θ from a 1-D fit on the optimal observable q_i
 - -Or possibly a 2-D fit on (q_i, D_i) including the pre-selection classifier D_i

Some of the many limitations of this approach

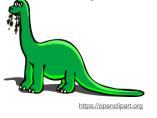
- MC weight derivative depend on θ : coupling fits easier than mass fits
- I ignored systematic errors
- I only discussed fits of a single physics parameter at a time
- But I still find this approach better than maximizing an AUC...

(Note: I did not try a real measurement – I did a few tests with a toy model, but I am not presenting them today)



Weight derivative regressors and their training

(a frequentist dinosaur's view of Machine Learning)



Classic ML problem: create a model $q(\mathbf{x})=R_{\gamma}(\mathbf{x})$ to predict the value of $\gamma(\mathbf{x})$ in a multi-dimensional space of variables \mathbf{x}

Choosing a ML methodology mainly implies two choices:

1. The shape of the function $R_{\gamma}(x)$:

i.e. how we choose to model $\gamma(\mathbf{x})$

Examples: decision tree (sparsely uniform), neural network (sigmoids), linear discriminant

I focus on **Decision Trees** because of the similarities to binned distribution fits

2. The training metric: a "distance" of $R_{\gamma}(\mathbf{x}_i)$ to $\gamma(\mathbf{x}_i)$ or γ_i to minimize, or a property of $R_{\gamma}(\mathbf{x}_i)$ to maximize Examples: Gini, Shannon entropy/information, MSE

I suggest to use I_{θ} or FIP both for training and for evaluation

Event selection and partitioning: a blurred boundary

(1) The scoring classifier D for signal/background discrimination is related to the average purity ρ(x): it would be a pity to use it only for a yes/no decision It can be used both for measuring cross-sections (1-D fit of D) or for measuring a mass or coupling (2-D fit against another variable)

Use the scoring classifier D to partition events, not only to accept or reject events



(2) Signal events with zero or low sensitivity to θ and background events are equally irrelevant

Separating signal events with high sensitivity to θ from background events

is as important as

Separating signal events with high sensitivity to θ from signal events with low sensitivity to θ

Fisher information (about a parameter θ)

Fisher information I_θ is a useful concept because

F. James, Statistical Methods in Experimental Physics, 2nd edition, World Scientific (2006).

- 1. It refers to the parameter θ that is being measured
- 2. It is additive: the information from independent measurements adds up
- 3. The higher the information I_{θ} , the lower the error $\Delta\theta$ achievable on θ

Cramer-Rao lower bound CRLB (lowest achievable variance $\Delta\theta^2$)

$$(\Delta \hat{\theta})^2 = \operatorname{var}(\hat{\theta}) \ge \frac{1}{\mathcal{I}_{\theta}}$$

- Some estimators achieve the CRLB and are called efficient
 - Example: a maximum likelihood fit (given the event counts in a given partitioning scheme)
- In the following **I** will express statistical error $\Delta heta$ in terms of information I $_{ heta}$

i.e. I will treat errors $\Delta\theta$ and information I_{θ} as equivalent concepts

$$\mathcal{I}_{\theta} = \frac{1}{(\Delta \theta)^2}$$

HEP cross-section in a counting experiment

- Measurement of a total cross-section σ_s in a counting experiment
- A distribution fit with a single bin
- Well-known since decades if final goal is to minimize statistical error Δσ_s
 - Maximise $\varepsilon_s^* \rho$ ("common knowledge" in the LEP2 experiments) \rightarrow "FIP1"
 - NB: This metric only makes sense for this specific HEP optimization problem!

$$\mathcal{I}_{\sigma_{s}} = \frac{1}{(\Delta \sigma_{s})^{2}} = \frac{1}{\sigma_{s}^{2}} \epsilon_{s} \varrho S_{\text{tot}} = \frac{1}{\sigma_{s}^{2}} \left(\frac{S_{\text{sel}}^{2}}{S_{\text{sel}} + B_{\text{sel}}} \right)$$

$$\mathcal{I}_{\sigma_{s}}^{(\text{ideal})} = \frac{S_{\text{tot}}}{\sigma_{s}^{2}}, \text{ if } \varrho = 1 \text{ and } \epsilon_{s} = 1$$

$$FIP_{1} = \frac{\mathcal{I}_{\sigma_{s}}}{\mathcal{I}_{\sigma_{s}}^{(\text{ideal})}} = \epsilon_{s} \varrho$$

By the way: ρ/ϵ_s =1 where $\partial FIP1/\partial \rho$ = $\partial FIP1/\partial \epsilon_s$ (just like for F1)

A brief comparison of MD, IR and HEP

Medical Diagnostics

- All patients are important, both truly ill (TP) and truly healthy (TN)
- e.g. ACC metric depends on all four categories: average over TP+TN+FP+FN

$ACC = \frac{TP + TN}{TP + TN + FP + FN}$

Information Retrieval

- Based on qualitative distinction between "relevant" and "non relevant" documents
- e.g. F1 metric <u>does not depend on True Negatives</u>
 - Rejected "irrelevant" documents are utterly irrelevant

$$F_1 = \frac{2 \text{ TP}}{2 \text{ TP} + \text{FP} + \text{FN}}$$

HEP (cross section measurement by counting)

- Based on qualitative distinction between signal and background
- e.g. FIP1 metric <u>does not depend on True Negatives</u>

events are rejected

Measured cross section cannot depend on how many background events are rejected

HEP is more similar to Information Retrieval than to Medical Diagnostics (qualitative asymmetry between positives and negatives)

Invariance under TN change is only one of many useful symmetries to analyse [Sokolova-Lapalme, Luque et al.]

M. Sokolova, G. Lapalme, A Systematic Analysis of Performance Measures for Classification Tasks, Information Processing and Management 45 (2009) 427. doi:10.1016/j.ipm.2009.03.002

A. Luque, A Carrasco, A. Martin, J. R. Lama, Exploring Symmetry of Binary Classification Performance Metrics, Symmetry 11 (2019) 47. doi:10.3390/sym11010047.



HEP: cross section in a counting experiment

(maximize FIP1 – the AUC is misleading!)

To minimize the statistical error $\Delta \sigma$:

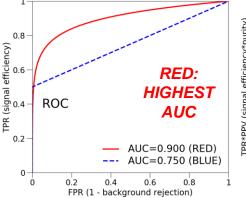
Maximize
$$FIP_1 = \epsilon_s \varrho$$

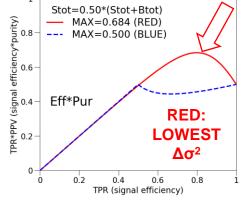
Choice between two classifiers is simple:

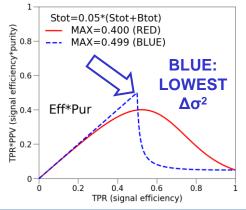
- Determine max $(\varepsilon_s \times \rho)$ for each
- Choose the classifier with the higher max

NB1: The choice depends on prevalence [which is fixed by physics and approximately known in advance]

NB2: AUC is misleading and irrelevant in this case







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

Choice of operating point is simple:

- Plot $\varepsilon_s \times \rho$ as a function of ε_s
- Choose the point where $\varepsilon_s \times \rho$ is maximum

But there are better ways than a counting experiment to measure a total cross section in this case...

HEP: cross section by a fit to the score distribution

Use the scoring classifier D to partition events, not to accept or reject events

This is the most common method to measure a total cross section (example: a BDT or NN output fit)

Keep all Stot events and partition them in K bins

$$\text{FIP}_2 = \frac{\mathcal{I}_{\sigma_s}}{\mathcal{I}_{\sigma_s}^{(\text{ideal})}} = \frac{\sum_k s_k \rho_k}{\sum_k s_k} = \frac{\sum_k s_k^2 / n_k}{\sum_k s_k} = \frac{\sum_k n_k \rho_k^2}{\sum_k s_k}$$

There is a benefit in partitioning events into subsets with different purities because

$$\Delta \mathcal{I}_{\sigma_s} = \frac{n_1 n_2}{n_1 + n_2} (\rho_1 - \rho_2)^2$$

Better than a counting experiment for two reasons

- All events are used, none are rejected
- Those which were previously in a single bin are now subpartitioned



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

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

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

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

Compare FIP2(ROC) to AUC

$$AUC = \int_0^1 \epsilon_s d\epsilon_b = 1 - \int_0^1 \epsilon_b d\epsilon_s$$

FIP2 from the PRC:

$$S_{\text{sel}} = S_{\text{tot}} \epsilon_s$$

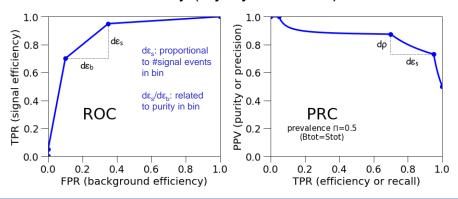
$$S_{\text{sel}} = S_{\text{tot}} \epsilon_s$$

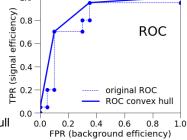
$$S_{\text{sel}} = S_{\text{tot}} \left(\frac{1}{\rho} - 1\right) \Longrightarrow s_i = dS_{\text{sel}} = S_{\text{tot}} \left[d\epsilon_s \left(\frac{1}{\rho} - 1\right) - \epsilon_s \frac{d\rho}{\rho^2}\right] \Longrightarrow \rho_i = \frac{\rho}{1 - \frac{\epsilon_s}{\rho} \frac{d\rho}{d\epsilon_s}} \Longrightarrow \text{FIP2} = \int_0^1 \frac{\rho \, d\epsilon_s}{1 - \frac{\epsilon_s}{\rho} \frac{d\rho}{d\epsilon_s}}$$

Compare FIP2(PRC) to AUCPR

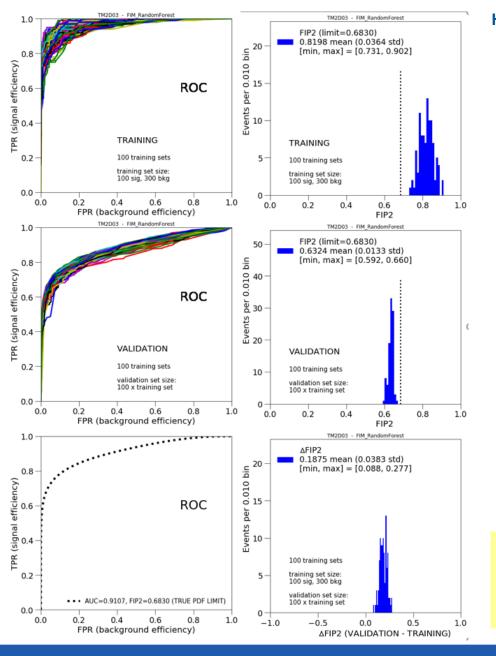
$$AUCPR = \int_0^1 \rho \, d\epsilon_s$$

- 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)



HEP estimation of parameter θ in a binned distribution fit

FIP2^(max) example (and overtraining)

FIP2 is a metric in [0,1]
but the detector resolution
effectively determines a FIP2^(max) < 1



Fisher information I_{θ} about θ (statistical errors)

For a given partitioning scheme with K bins (n_k is the number of selected events in bin k)

Bin-by-bin sensitivity to θ

$$\mathcal{I}_{\theta} = \frac{1}{(\Delta \theta)^2} = \sum_{k=1}^{K} \frac{1}{(\Delta \theta)_k^2} = \sum_{k=1}^{K} n_k \left(\frac{1}{n_k} \frac{\partial n_k}{\partial \theta} \right)^2$$

Statistical errors: information adds up

Each bin is an independent measurement with error $(\Delta\theta)_k = \left(\frac{\partial n_k}{\partial \theta}\right)^{-1} \Delta n_k = \left(\frac{\partial n_k}{\partial \theta}\right)^{-1} \sqrt{n_k}$

(Combination more complex with systematic errors, or for searches)



Optimal partitioning

$$\mathcal{I}_{\theta} = \frac{1}{(\Delta \theta)^2} = \sum_{k=1}^{K} \frac{1}{(\Delta \theta)_k^2} = \sum_{k=1}^{K} n_k \left(\frac{1}{n_k} \frac{\partial n_k}{\partial \theta} \right)^2$$

Is there a benefit (information inflow) in splitting bin 0 into two bins 1, 2 with $n_0 = n_1 + n_2$?

$$\begin{split} \Delta \mathcal{I}_{\theta} &= \frac{1}{n_1} \left(\frac{\partial n_1}{\partial \theta} \right)^2 + \frac{1}{n_2} \left(\frac{\partial n_2}{\partial \theta} \right)^2 - \frac{1}{n_1 + n_2} \left(\frac{\partial (n_1 + n_2)}{\partial \theta} \right)^2 \\ &= \frac{n_1 n_2}{n_1 + n_2} \left[\left(\frac{1}{n_1} \frac{\partial n_1}{\partial \theta} \right) - \left(\frac{1}{n_2} \frac{\partial n_2}{\partial \theta} \right) \right]^2 \end{split}$$

Information increases if the two new bins have different sensitivities to θ

$$\Delta \mathcal{I}_{\theta} > 0 \iff \left(\frac{1}{n_1} \frac{\partial n_1}{\partial \theta}\right) \neq \left(\frac{1}{n_2} \frac{\partial n_2}{\partial \theta}\right)$$

Goal of a distribution fit: partition events into subsets with different bin-by-bin sensitivities to θ

Signal and background are not dichotomous classes

(with one exception: cross section measurements)

Background events by definition are insensitive to θ Signal events may have positive, zero or negative sensitivity

θ: mass, coupling NON-DICHOTOMOUS

$$\gamma_i = \left(\frac{1}{w_i} \frac{\partial w_i}{\partial \theta}\right) = 0, \quad \text{if } i \in \{\text{Background}\}$$

$$\gamma_i = \left(\frac{1}{w_i} \frac{\partial w_i}{\partial \theta}\right) \in \{-\infty, +\infty\}, \quad \text{if } i \in \{\text{Signal}\}\$$

$$\delta_i = \begin{cases} 1 & \text{if } i \in \{\text{Signal}\}\\ 0 & \text{if } i \in \{\text{Background}\} \end{cases}$$

The distinction between signal events with low ($|\gamma_i|$ ~0) sensitivity and background events is blurred (example: events far from an invariant mass peak)

Changing the signal cross section ~is a global rescaling of all differential distributions $s_k(\sigma_s) = \frac{\sigma_s}{\sigma_{s \text{ rof}}} \times s_k(\sigma_{s, \text{ref}})$

In a cross section measurement
All background events are equivalent to one another
All signal events are equivalent to one another

$$\gamma_i = \frac{1}{\sigma_s} \delta_i = \begin{cases} \frac{1}{\sigma_s} & \text{if } i \in \{\text{Signal}\}, \\ 0 & \text{if } i \in \{\text{Background}\}, \end{cases} \quad \text{if } \theta \equiv \sigma_s$$

 θ : cross section σ_s DICHOTOMOUS



FIP1 and FIP2 revisited

FIP_{sha}=1 for both

(dichotomous, all signal events are equivalent)

$$FIP_{3} = \frac{\sum_{k=1}^{K} s_{k} \rho_{k} \phi_{k}^{2}}{\sum_{i=1}^{S_{\text{tot}}} \gamma_{i}^{2}} = FIP_{\text{eff}} \times FIP_{\text{sha}} \times FIP_{\text{pur}}$$

$$= \frac{\sum_{i=1}^{S_{\text{sel}}} \gamma_{i}^{2}}{\sum_{i=1}^{S_{\text{tot}}} \gamma_{i}^{2}} \times \frac{\sum_{k=1}^{K} s_{k} \phi_{k}^{2}}{\sum_{i=1}^{S_{\text{sel}}} \gamma_{i}^{2}} \times \frac{\sum_{k=1}^{K} s_{k} \rho_{k} \phi_{k}^{2}}{\sum_{k=1}^{K} s_{k} \phi_{k}^{2}}$$

$$FIP_{1} = \epsilon$$

$$FIP_{1} = \epsilon$$

$$FIP_{1} = \epsilon$$

$$FIP_{2} = \epsilon$$

$$FIP_{2} = \epsilon$$

$$FIP_1 = \epsilon_s \varrho$$

FIP1:

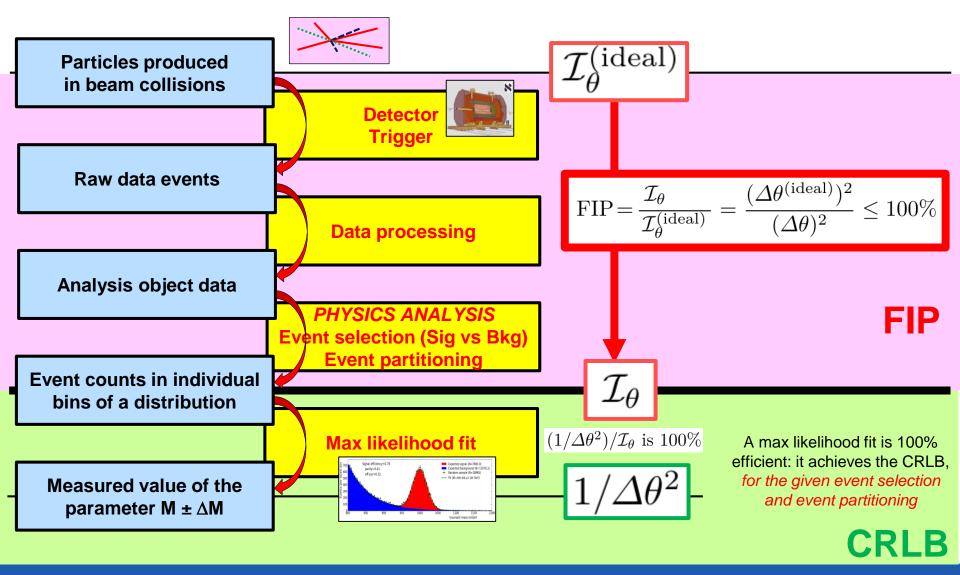
$$\mathsf{FIP}_{\mathsf{pur}} \!\!=\!\! \rho$$

$$\begin{aligned} \text{FIP}_2 = & \frac{\mathcal{I}_{\sigma_s}}{\mathcal{I}_{\sigma_s}^{(\text{ideal})}} = & \frac{\sum_k s_k \rho_k}{\sum_k s_k} = \frac{\sum_k s_k^2 / n_k}{\sum_k s_k} = \frac{\sum_k r_k}{\sum_k s_k} \end{aligned}$$

$$\begin{aligned} & \text{FIP2:} \\ & \text{FIP}_{\text{eff}} = 1 \\ & \text{FIP}_{\text{pur}} = \text{FIP2} \end{aligned}$$

$$\begin{aligned} \text{FIP}_2 = & \frac{\mathcal{I}_{\sigma_s}}{\mathcal{I}_{\sigma_s}^{(\text{ideal})}} = \frac{\sum_k s_k \rho_k}{\sum_k s_k} = \frac{\sum_k s_k^2 / n_k}{\sum_k s_k} = \frac{\sum_k n_k \rho_k^2}{\sum_k s_k} \end{aligned} \\ & \text{FIP}_3 = \frac{\sum_{k=1}^K s_k \rho_k \phi_k^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2} = \text{FIP}_{\text{eff}} \times \text{FIP}_{\text{sha}} \times \text{FIP}_{\text{pur}} \\ = \frac{\sum_{i=1}^K \gamma_i^2}{\sum_{i=1}^{S_{\text{tot}}} \gamma_i^2} \times \frac{\sum_{k=1}^K s_k \phi_k^2}{\sum_{i=1}^K \gamma_i^2} \times \frac{\sum_{k=1}^K s_k \rho_k \phi_k^2}{\sum_{k=1}^K s_k \rho_k \phi_k^2} \end{aligned}$$

From CRLB to Fisher Information Part (FIP)





Two optimization handles: event selection and partitioning

