The most beautiful line you can draw with Kalman filter

Valeriia (Lera) Lukashenko

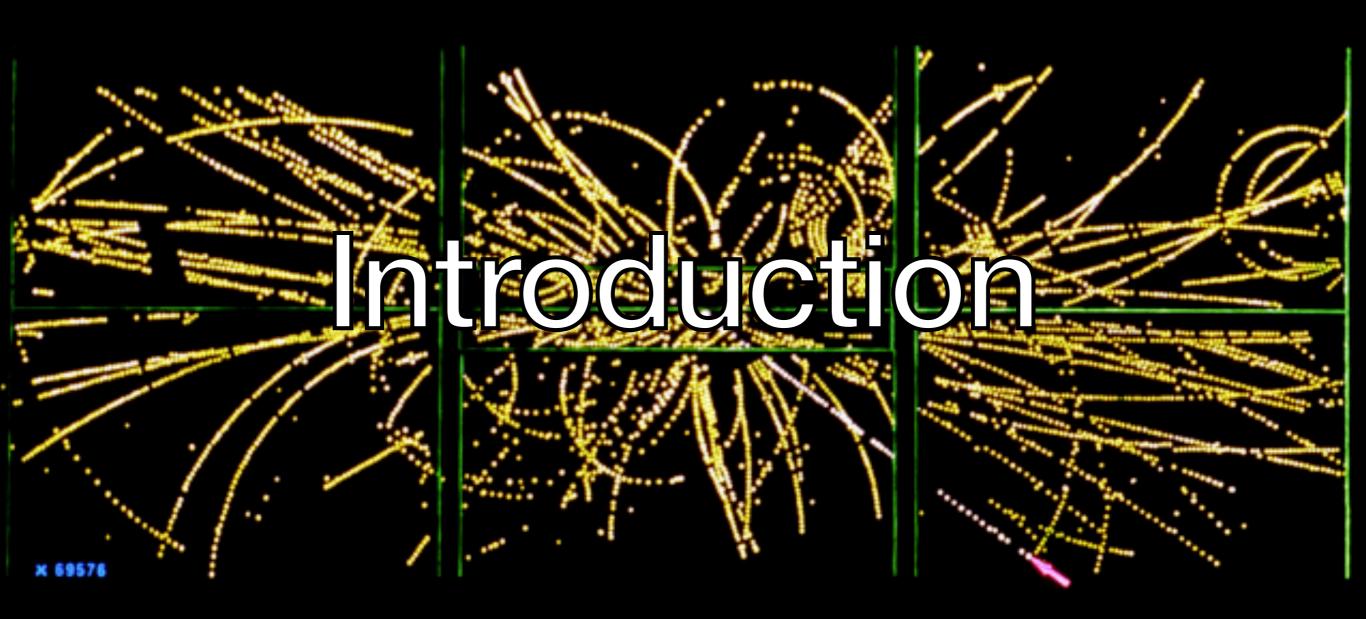
iCSC 2023

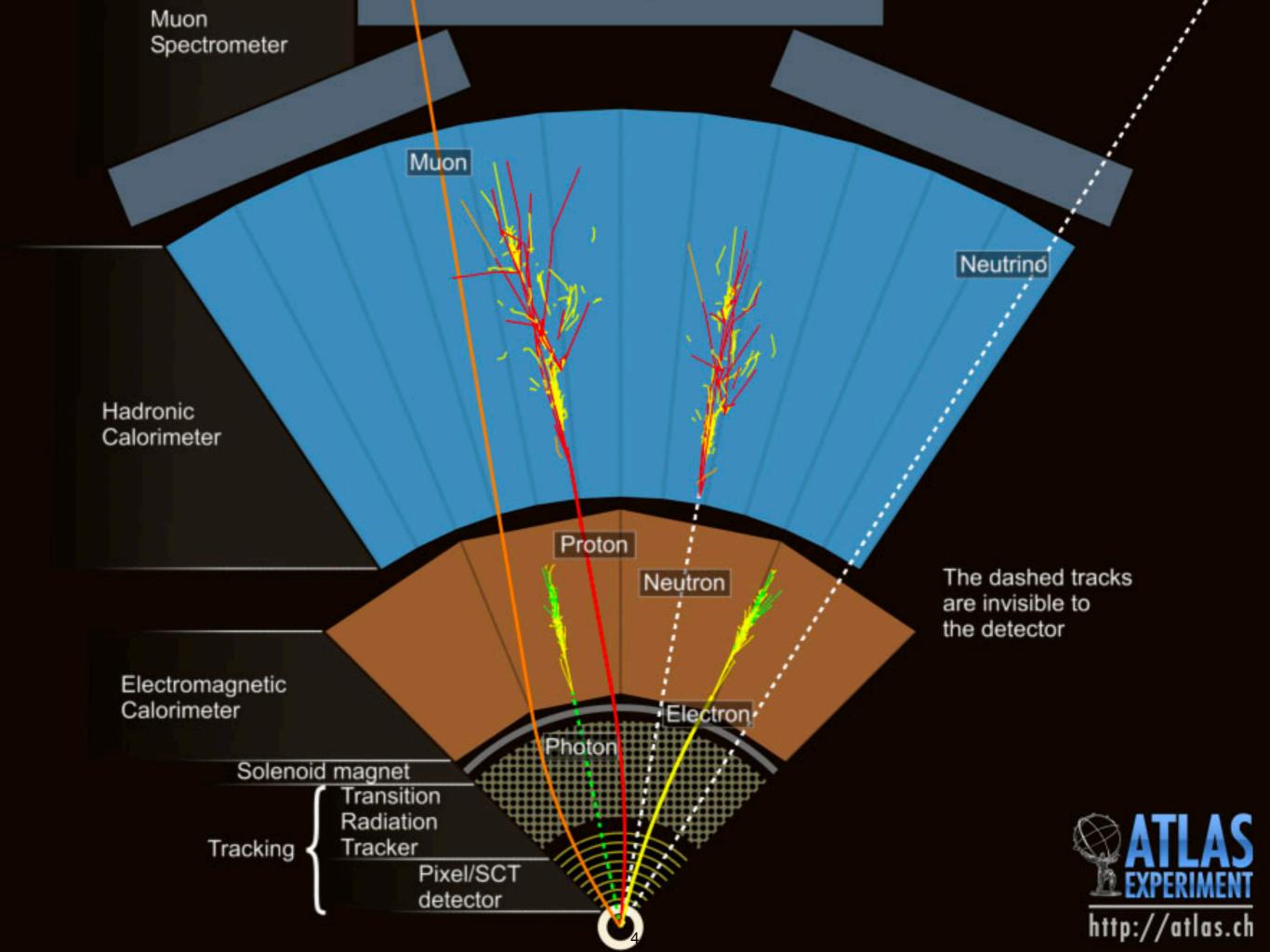
Based on/your read list

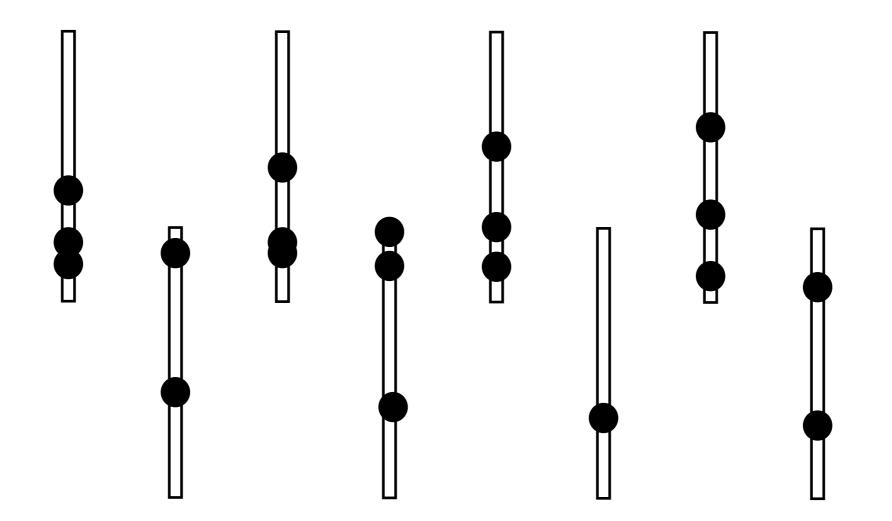
- Wouter Hulsbergen "Charged particle reconstruction and alignment" all the math can be found here
- Jeroen Van Tilburg "Track Simulation and reconstruction in LHCb" the to-go tracking thesis in LHCb, useful Kalman filter reference
- R.Frühwirth, A.Strandlie "Pattern Recognition, Tracking and Vertex Reconstruction" - the most full book on tracking I know of
- R.Frühwirth Application of Kalman Filtering to Tracking and Vertex Fitting

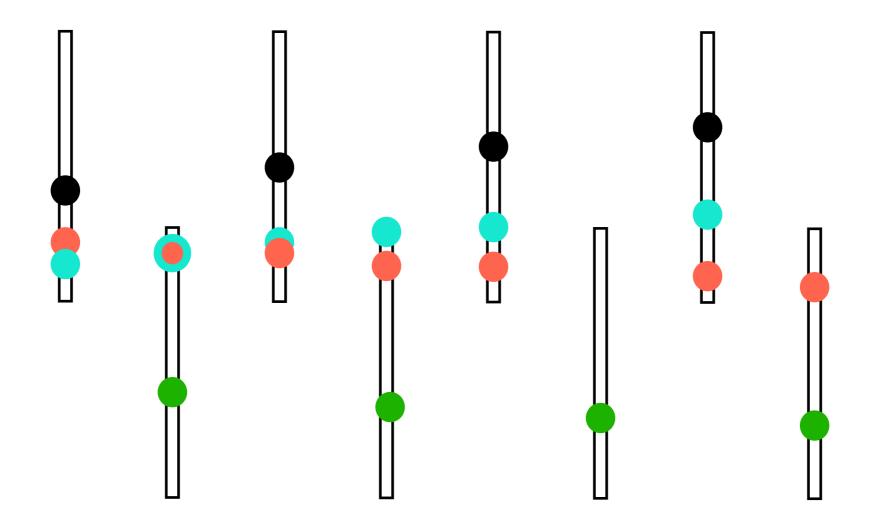
 eternal classics
- X. Ai, G. Mania, H.Gray, M.Kuhn, N. Styles <u>A GPU-based Kalman Filter for</u> <u>Track Fitting</u>

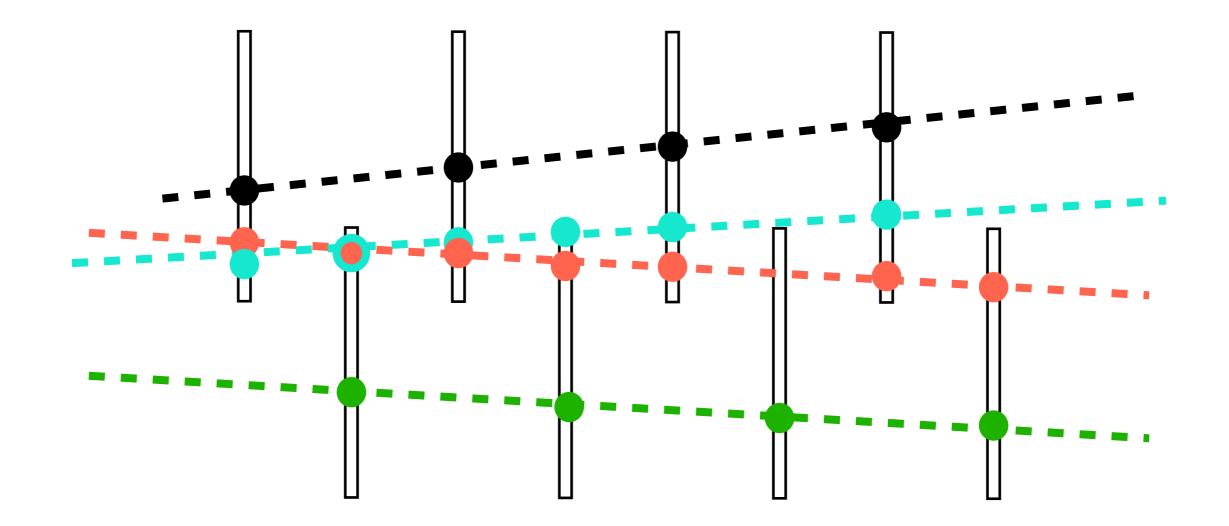
EVENT 2958. 1279.

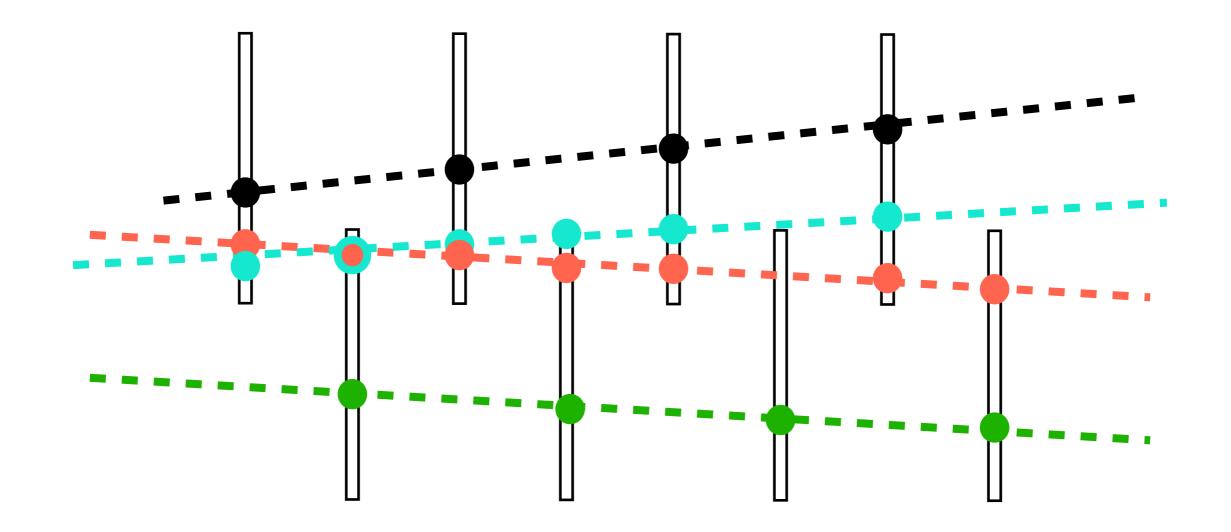






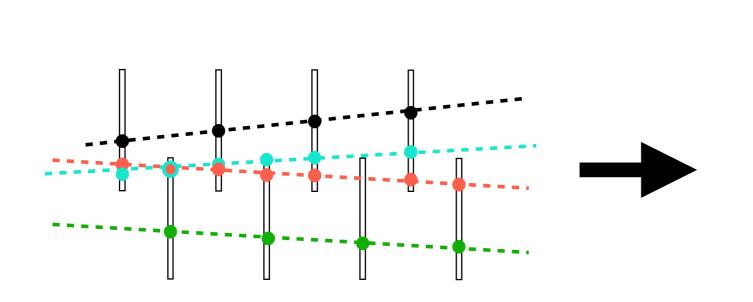


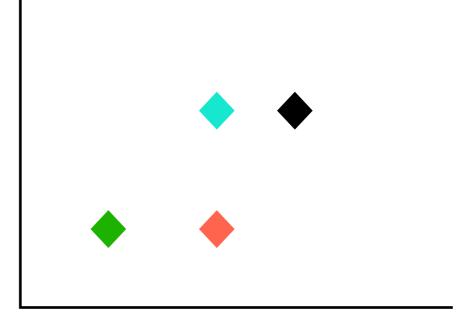




Which hit belongs to which track?

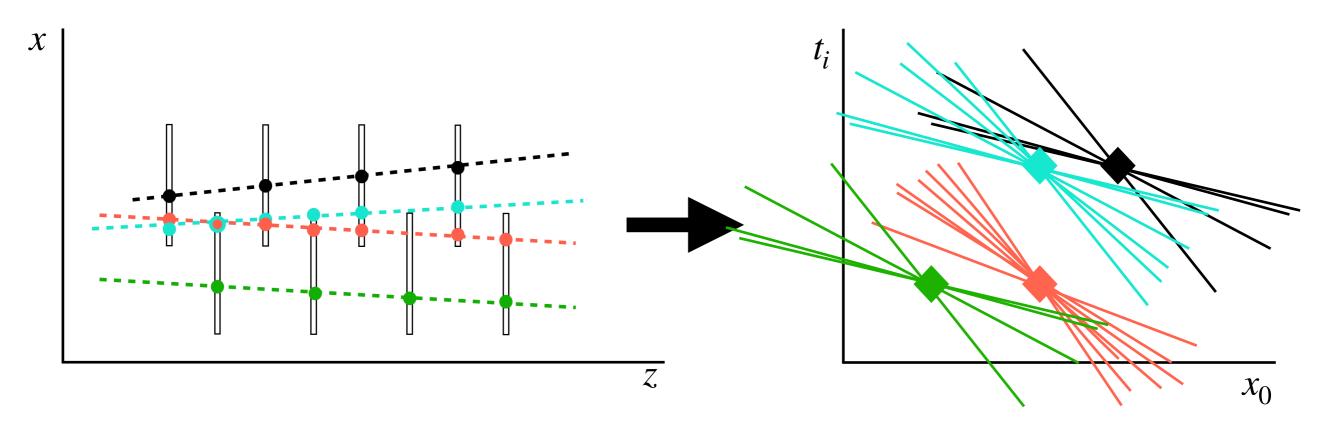
Which hit belongs to which track





classifier

Which hit belongs to which track

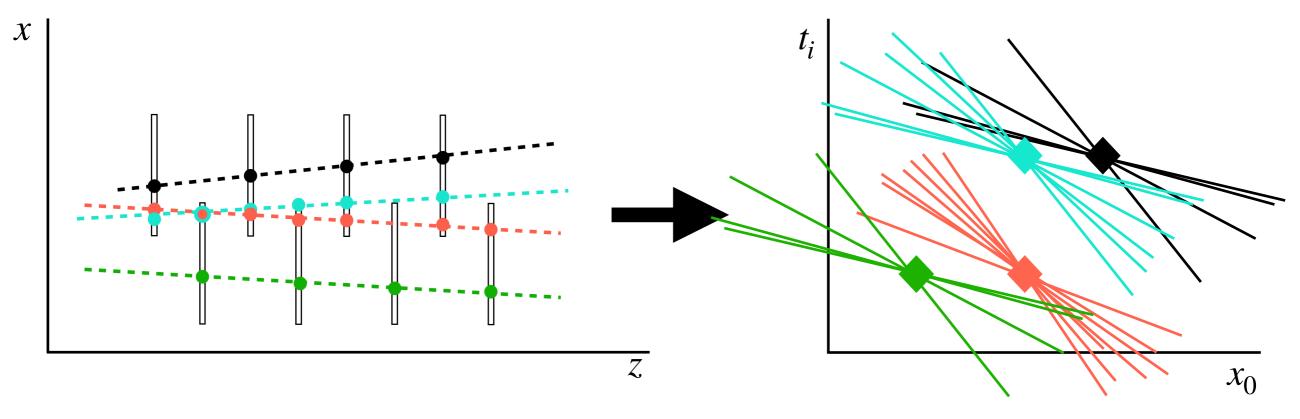


classifier

Hough transform

$$m_i(x,z) \to t_i = \frac{x - x_0}{z}$$

Which hit belongs to which track

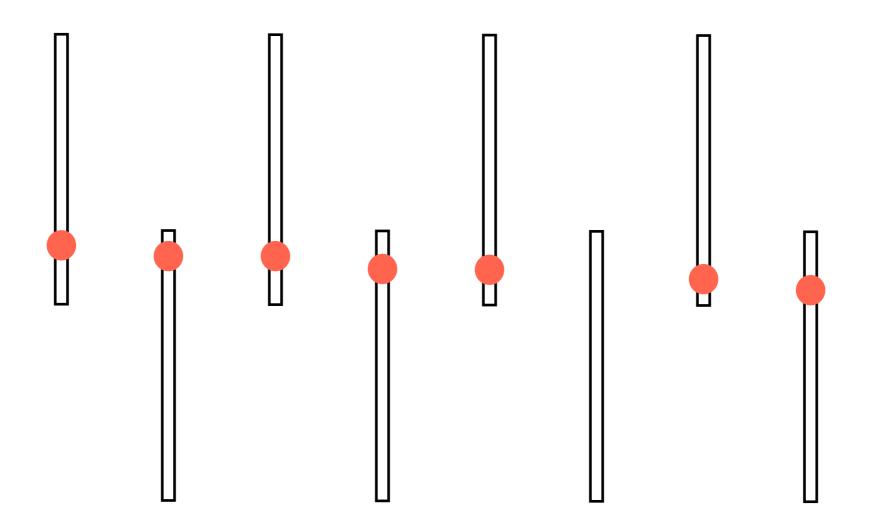


classifier

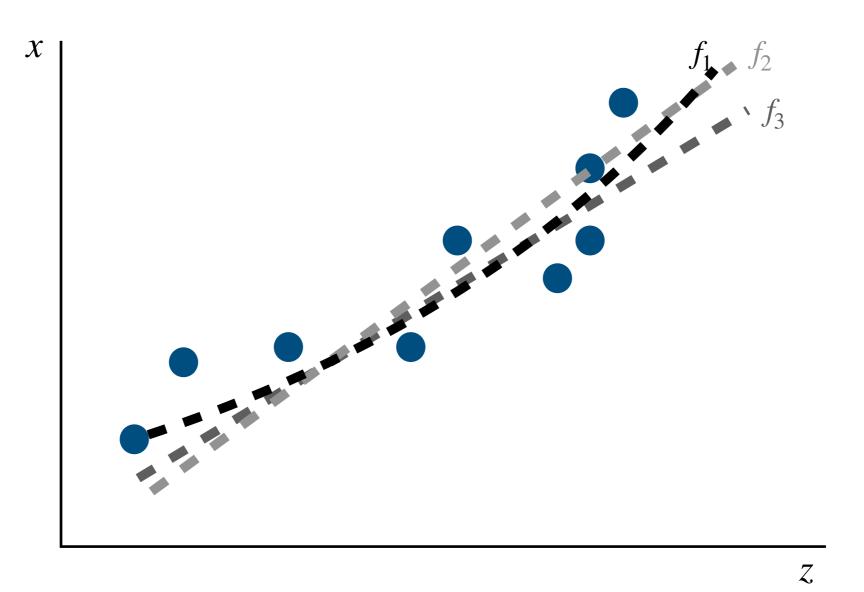
- machine learning
- "seeding" algorithm (local patter recognition)
- •etc.

How do I draw a line?

aka track fitting

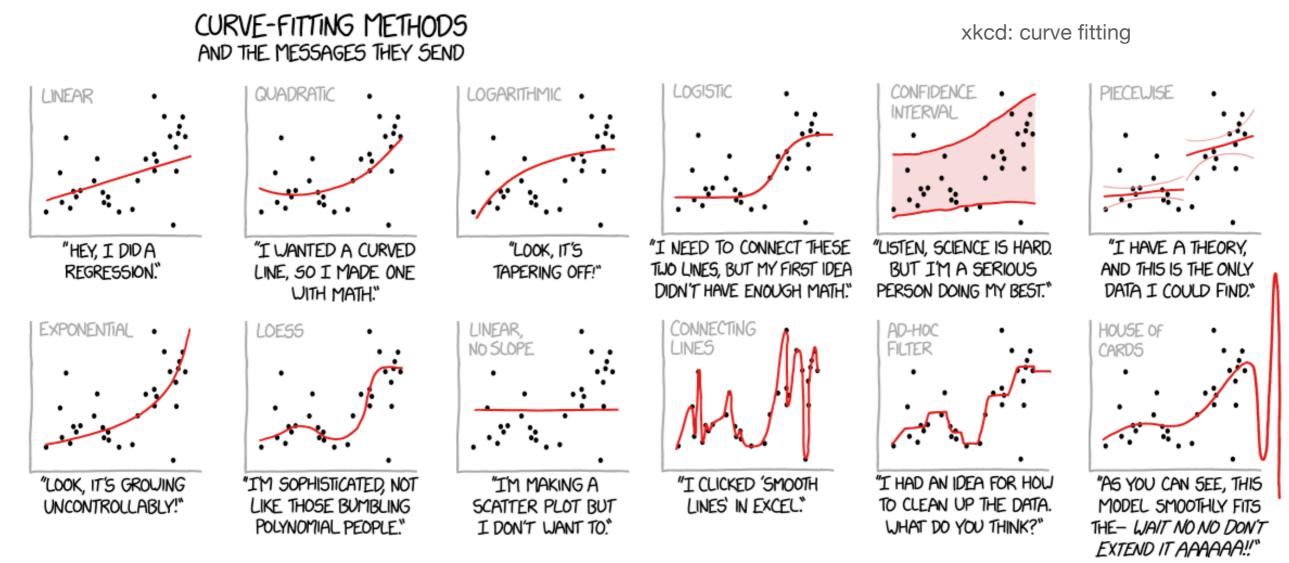


Reminder: fitting



$$f_1 = \sum_n \alpha_n z^n$$
 $f_2 = \sum_n \beta_n z^n$ $f_3 = \sum_n \gamma_n z^n$
fitting = estimating parameters of the model

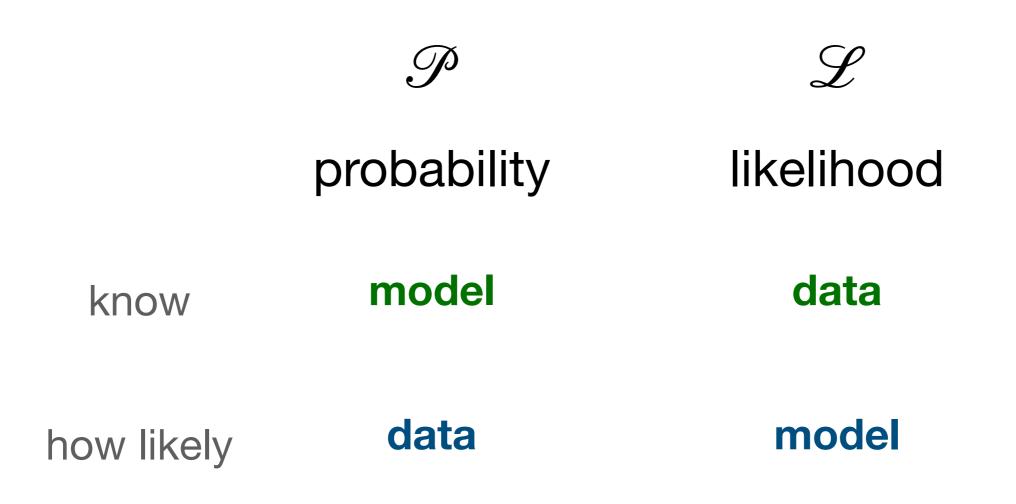
Reminder: fitting



two simple facts to spell out:

- choosing the model is purely subjective
- if model "fits" it does not mean it is "true"

Reminder: fitting



Reminder: fitting Maximum Likelihood Estimator

$$\begin{aligned} \mathscr{L}(\alpha; z) &= \prod_{i} \mathscr{P}(z_{i}; \alpha) \\ max(\mathscr{L}) \to \frac{d\mathscr{L}(\alpha; z)}{d\alpha} = 0 \to \hat{\alpha} \end{aligned}$$

Reminder: fitting Maximum Likelihood Estimator

$$ln\mathscr{L}(\alpha; z) = \sum_{i} ln\mathscr{P}(z_{i}; \alpha)$$
$$min(-\mathscr{L}) \to \frac{d(-ln\mathscr{L})(\alpha; z)}{d\alpha} = 0 \to \hat{\alpha}$$

- \sum is easier than \prod
- minimisation and maximisation are the same, but the convention is to represent maximum likelihood estimation via minimisation

Reminder: fitting Maximum Likelihood Estimator

$$ln\mathscr{L}(\alpha; z) = \sum_{i} ln\mathscr{P}(z_{i}; \alpha)$$
$$min(-\mathscr{L}) \to \frac{d(-ln\mathscr{L})(\alpha; z)}{d\alpha} = 0 \to \hat{\alpha}$$
$$V(\hat{\alpha}) = \sigma^{2} = \left[E\left(-\frac{\partial^{2}ln\mathscr{L}}{\partial\alpha^{2}}\right)\right]^{-1}$$

V is variance aka spread aka uncertainty

Reminder: fitting, example Least Square Estimator : χ^2

If $\mathscr{P}(z_i; \alpha) = \mathscr{N}(h_i(\alpha), \sigma_i)$, then

What I see What I expect $\sum_{i} ln \mathcal{P} \to \chi^{2} = \sum_{i} \left(\frac{z_{i} - h_{i}(\alpha)}{\sigma_{i}} \right)^{2}$

How good my vision is

$$\min\left(\sum_{i} \ln\mathcal{P}\right) \Rightarrow \frac{d\chi^2}{d\alpha} = 0 \to \hat{\alpha}$$





What I see What I expect

$$\chi^2 = \sum_{i} \left(\frac{z_i - h_i(\alpha)}{\sigma_i} \right)^2 = \left(z - h(\alpha) \right)^T (\sigma^2)^{-1} \left(z - h(\alpha) \right)$$

How good my vision is

tensor form





What I see What I expect

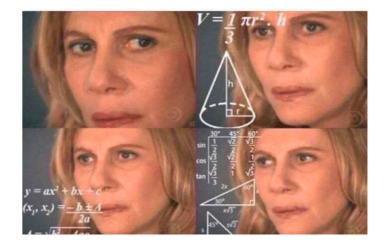
$$\chi^2 = \sum_{i} \left(\frac{z_i - h_i(\alpha)}{\sigma_i} \right)^2 = \left(z - h(\alpha) \right)^T V^{-1} \left(z - h(\alpha) \right)$$
tensor form

How good my vision is

 $h(\alpha) = h_0 + H\alpha$

$$H = \frac{dh(\alpha)}{d\alpha}$$

χ^2 formalism Solution



 $\hat{\alpha} = (H^T V^{-1} H)^{-1} H^T V^{-1} (z - h_0)$

Are you worried about anything in this formula? (note variance matrix - is a positive definite and diagonal matrix by definition)

$$h(\alpha) = h_0 + H\alpha$$
 $H = \frac{dh(\alpha)}{d\alpha}$

χ^2 formalism Solution



$$\hat{\alpha} = (H^T V^{-1} H)^{-1} H^T V^{-1} (z - h_0)$$

$$h(\alpha) = h_0 + H\alpha$$
 $H = \frac{dh(\alpha)}{d\alpha}$

χ^2 formalism Solution



$$\hat{\alpha} = (H^{T}V^{-1}H)^{-1}H^{T}V^{-1}(z - h_{0})$$

$$\bigwedge$$

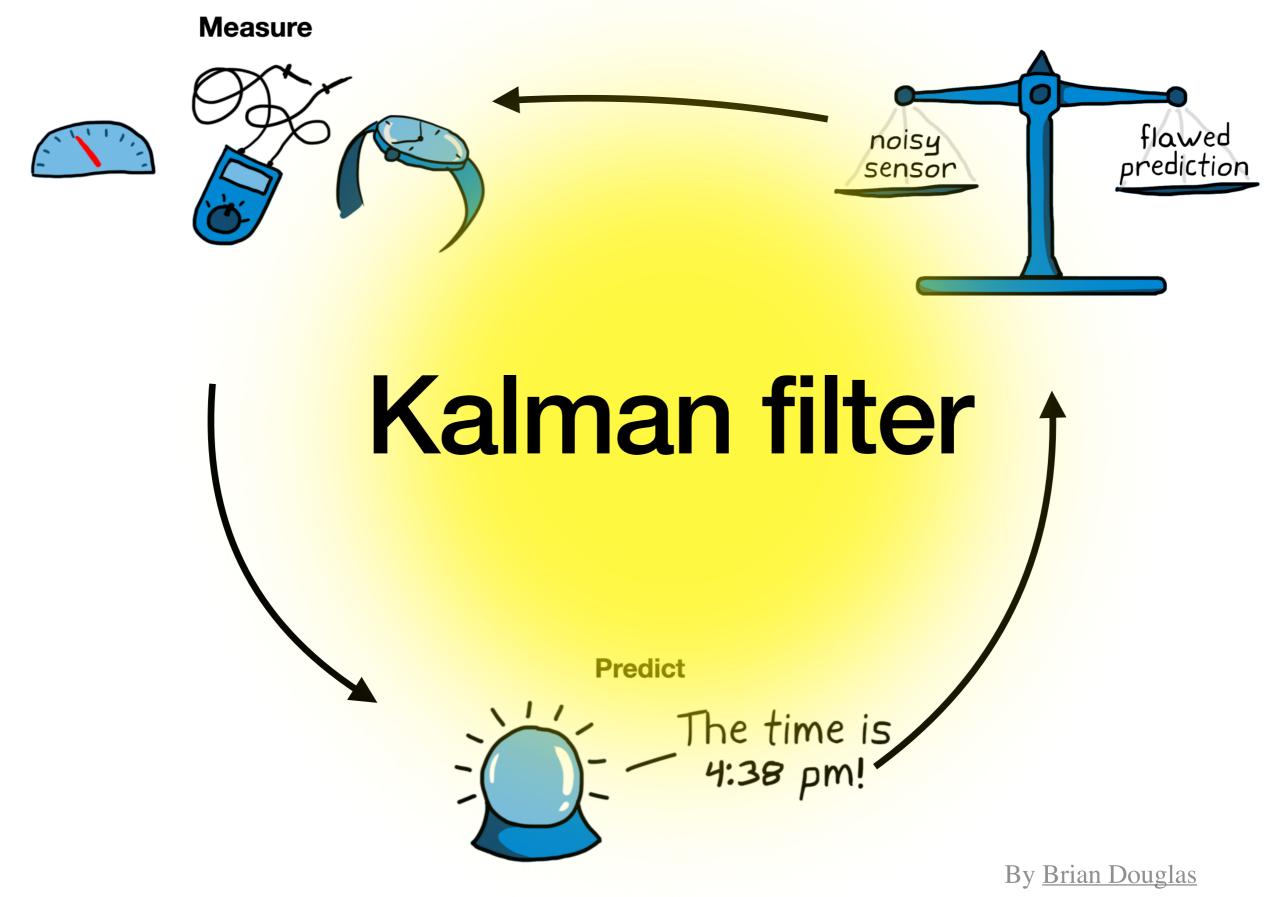
$$det(H^{T}V^{-1}H) \neq 0$$

$det(H^TV^{-1}H) = 0$: Underconstrained problem

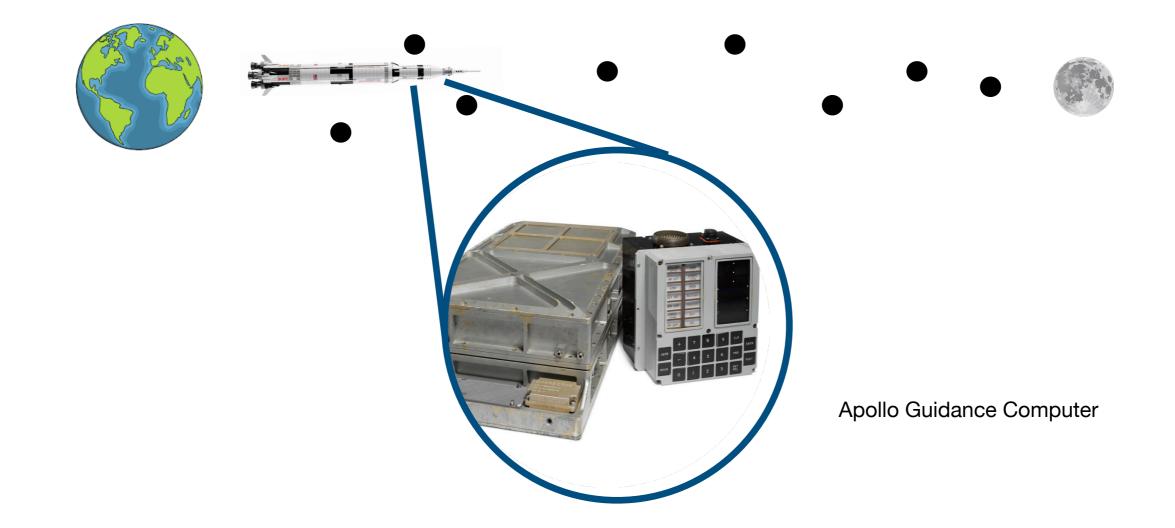
$$h(\alpha) = h_0 + H\alpha$$
 $H = \frac{dh(\alpha)}{d\alpha}$

 $det(H^T V^{-1} H) = 0$

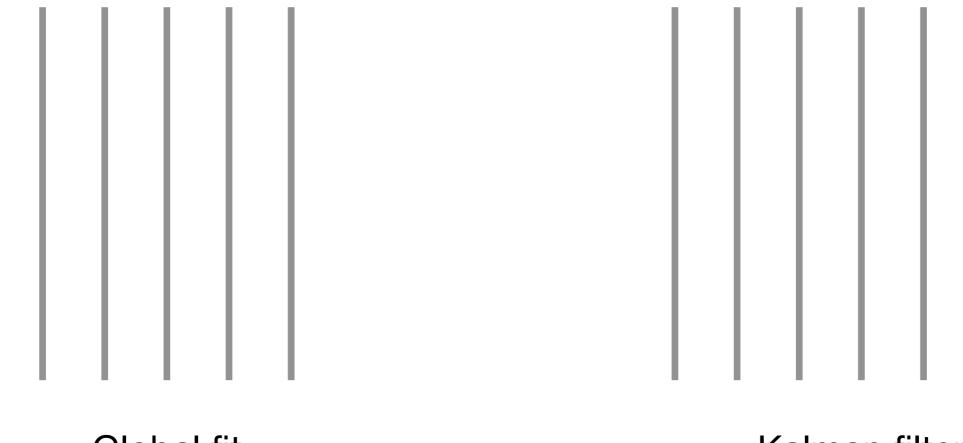
- some linear combination of elements of α have no finite variance \Rightarrow unconstrained degrees of freedom; can be isolated by diagonalizing the $H^T V^{-1} H$.
- the problem is always underconstrained for models with more parameters than data points



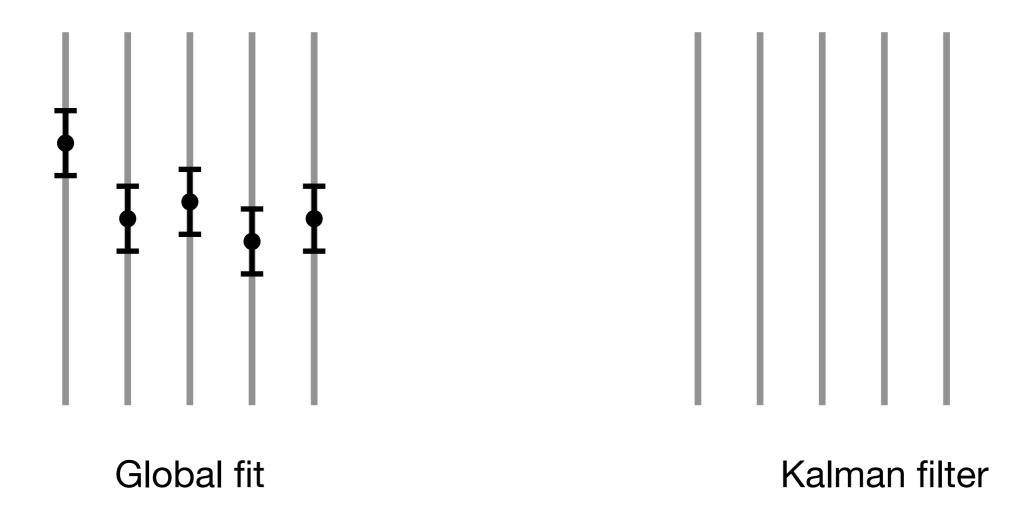
Apollo 11 mission

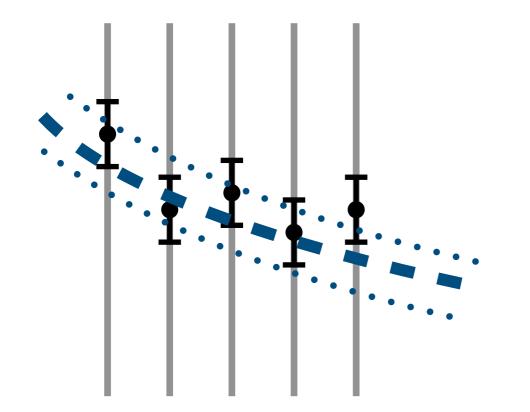


Problem: knowing trajectory of the spaceship with very limited computer resources and irregular measurements

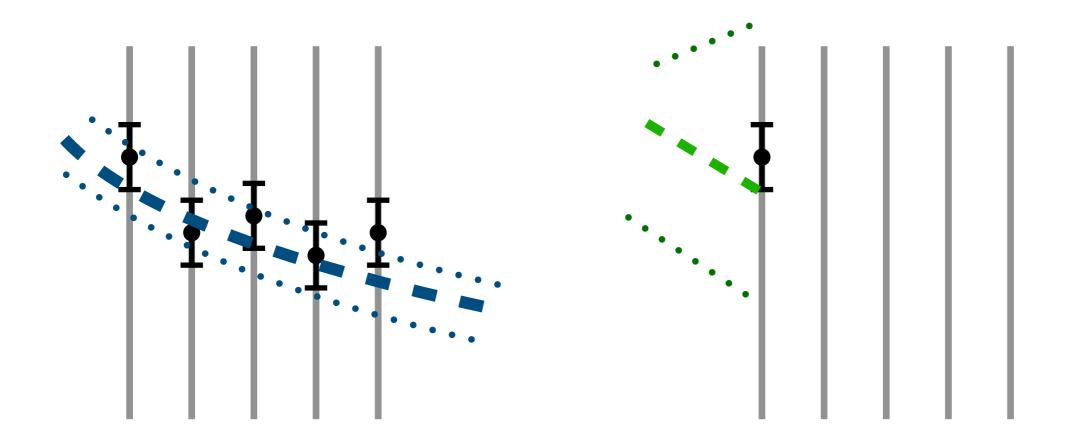


Global fit

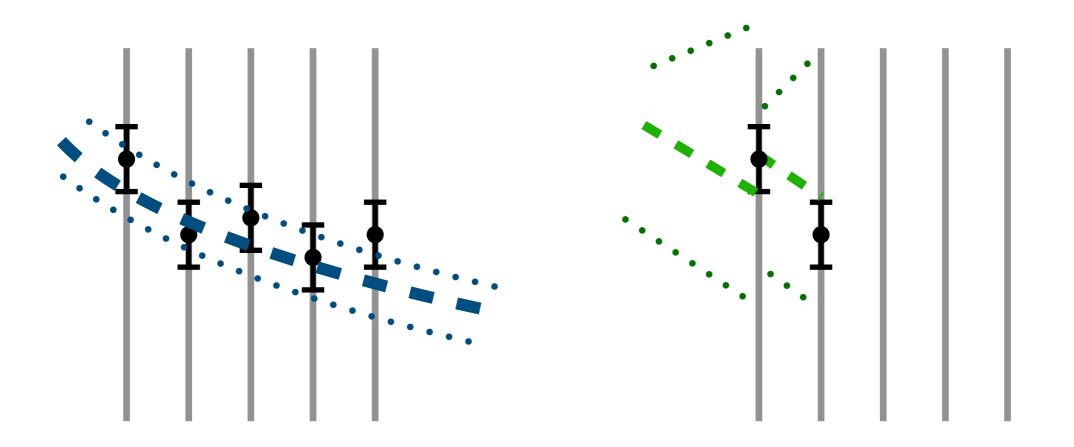




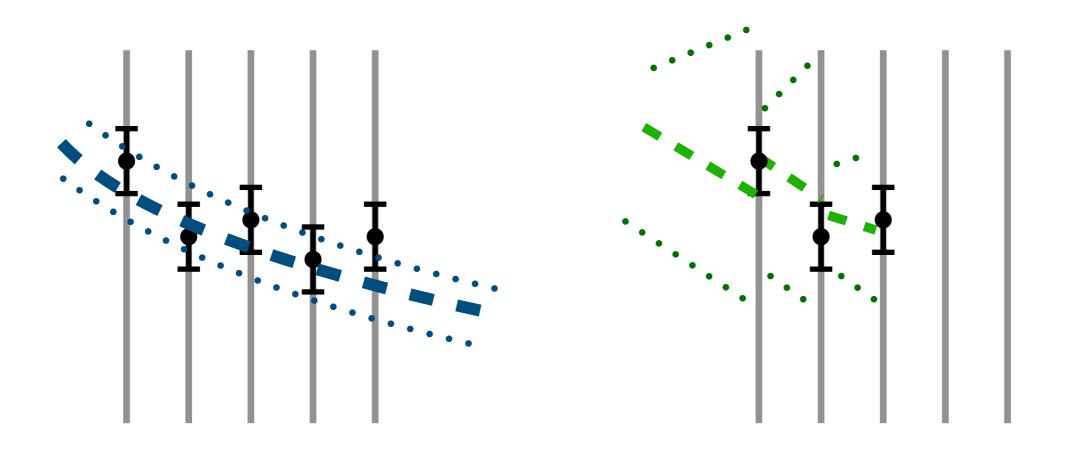
Global fit



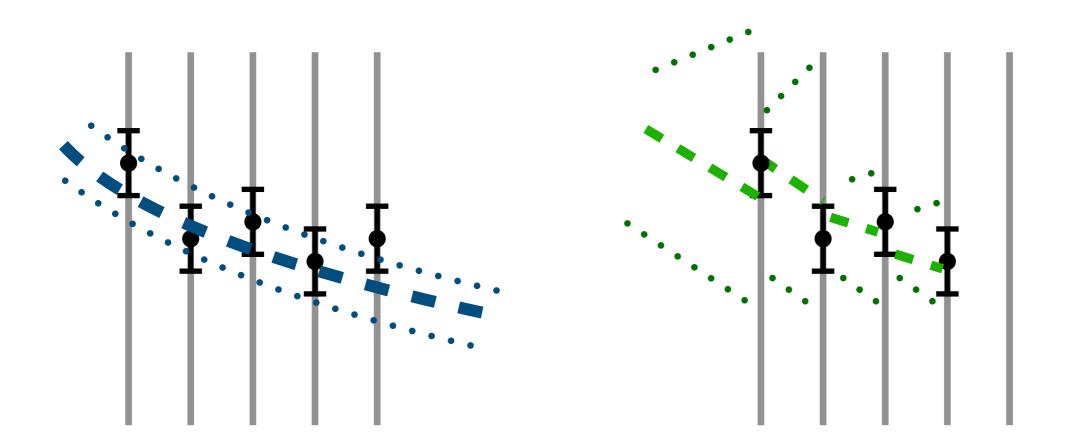
Global fit



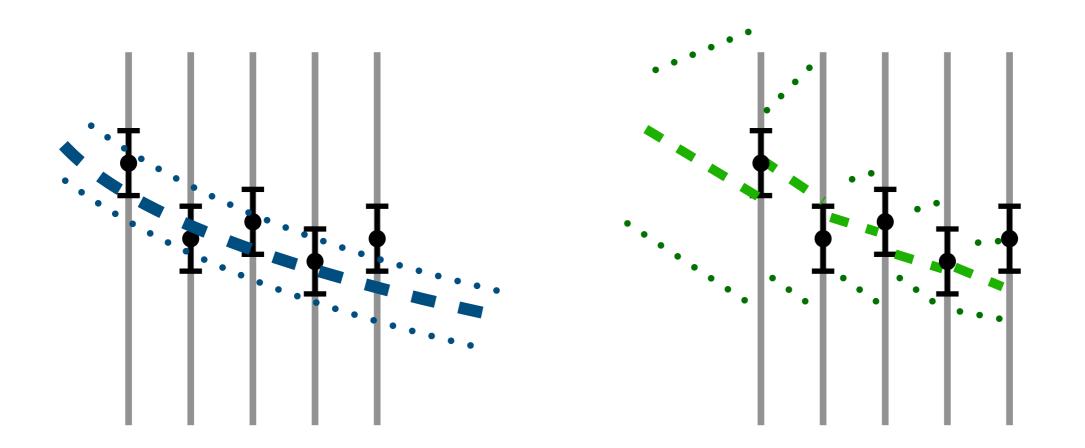
Global fit



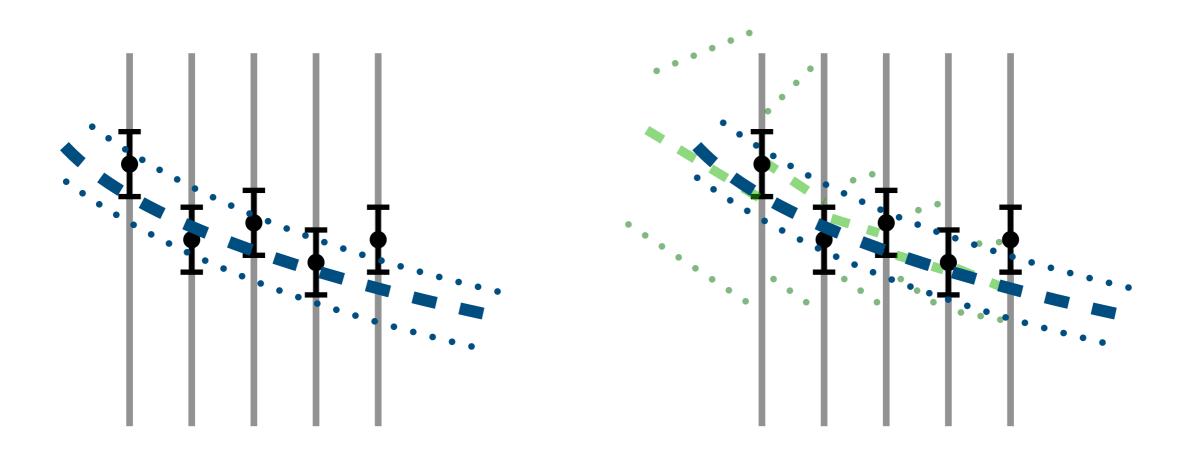
Global fit



Global fit

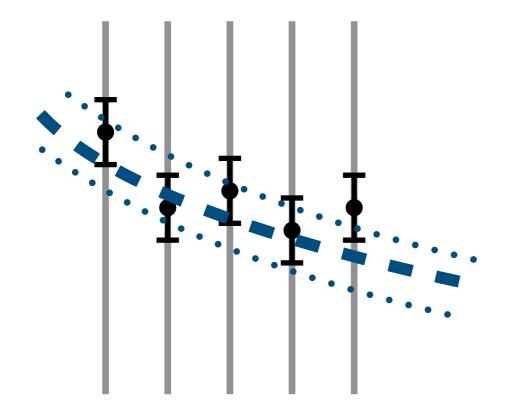


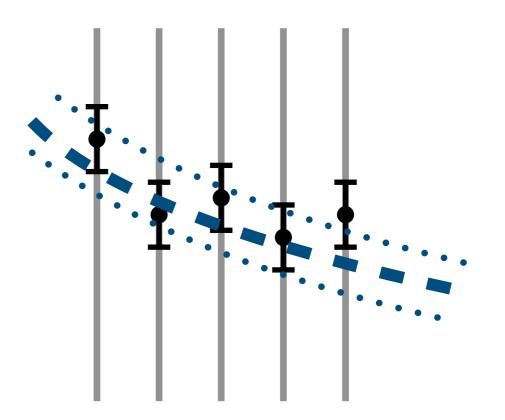
Global fit



Global fit

Kalman formalism





Global fit

Kalman filter

1 computation of *M*-equation system inversion of the $M \times M$ matrix M computations of 1-equation system inversion of the 1×1 matrix

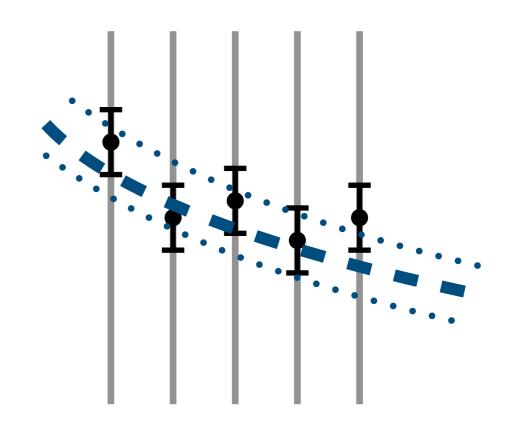
M - is number of measurement

Note: measurements might be not 1D

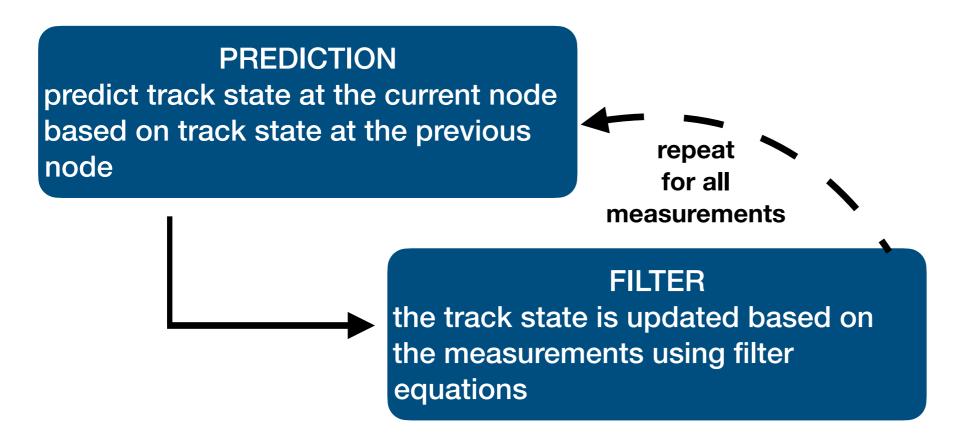
Kalman formalism

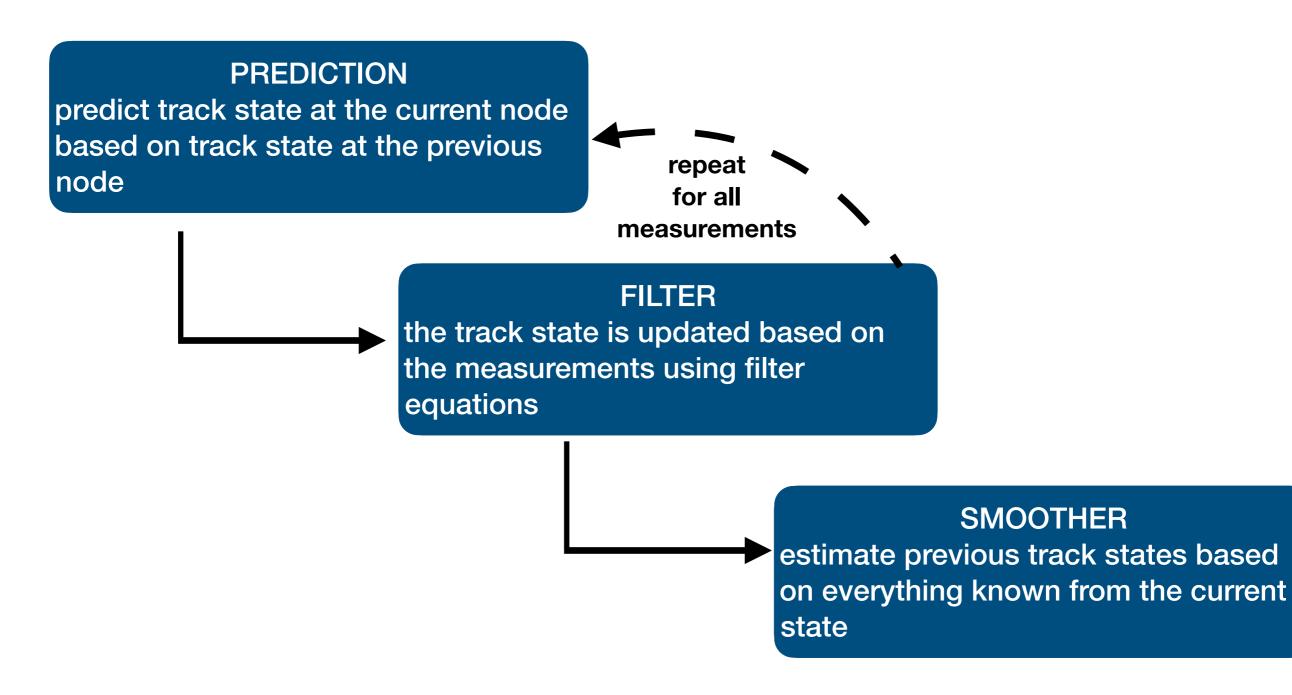
avoid inversion of $M \times M$ matrices easy to add noise and constraints

validity of linear approximation only last state benefits from all information



Kalman filter





Track fitter based on Kalman filter Time scale

Predict:

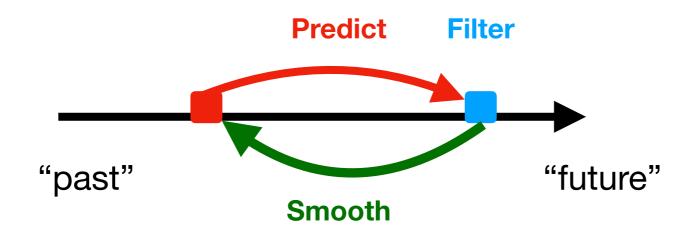
future state based on the current state

Filter:

current state based on the current and past measurements

Smoother:

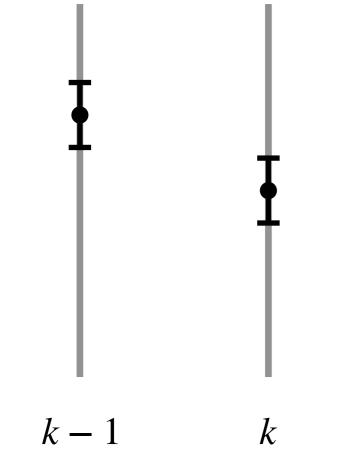
past states based on all measurements up to now



Prediction

PREDICTION

predict track state at the current node based on track state at the previous node



 α : track parameters C: track parameters variance

Prediction

 $\alpha_{k-1}; C_{k-1}$

PREDICTION

predict track state at the current node based on track state at the previous node

 α : track parameters *C*: track parameters variance

Prediction

 $\alpha_{k-1} + \frac{f_k(\alpha_{k-1})}{C_{k-1}}$

PREDICTION

predict track state at the current node based on track state at the previous node

Uses filtered state from the previous step of the filter

 α : track parameters C: track parameters variance Note: α is a vector

45

Prediction

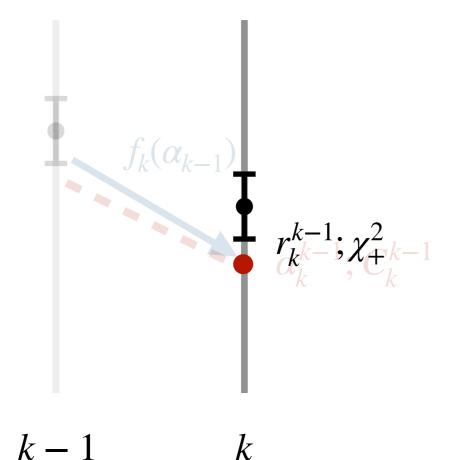
 $k-1 \qquad k$

PREDICTION

predict track state at the current node based on track state at the previous node

 α : track parameters C: track parameters variance f: propagation function

Prediction



PREDICTION

predict track state at the current node based on track state at the previous node

> Goal: minimize χ^2_+ $r_k^{k-1} = m_k - h_k(\alpha_k^{k-1})$

α: track parameters*m*: measurement*h*: projection function

Filter

k – 1

k

FILTER

the track state is updated based on the measurements using filter equations

Goal: minimize χ^2_+

$$\alpha_k = \alpha_k^{k-1} + K_k r_k^{k-1}$$
$$C_k = (1 - K_k H_k) C_k^{k-1}$$

gain matrix

α: track parameters*C*: track parameters variance

Gain matrix K_k

FILTER

the track state is updated based on the measurements using filter equations

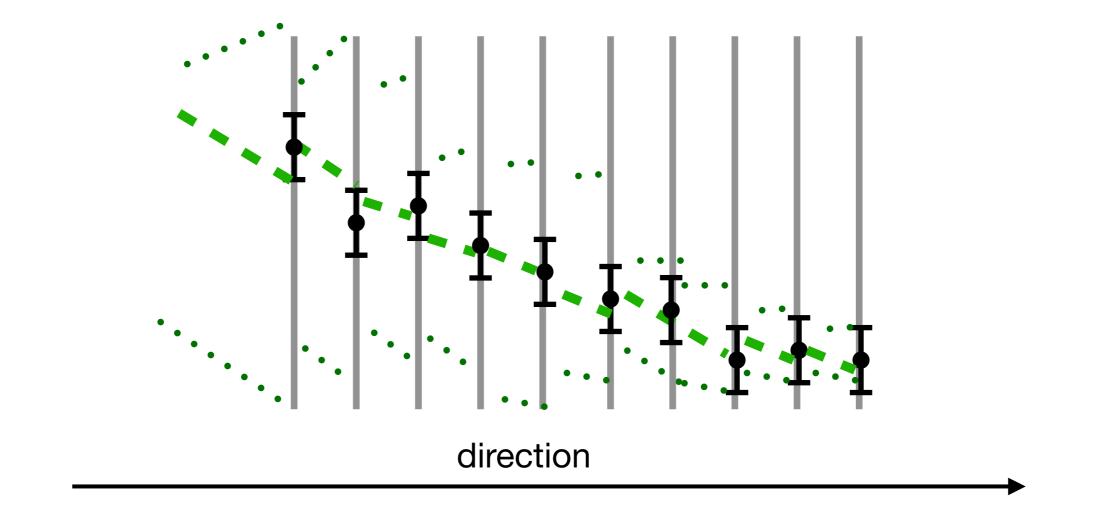
Gain matrix tells us how much should our prediction change if adding the information about the measurement aka the weight of the prediction versus measurement

Very precise measurements:

Very precise prediction:

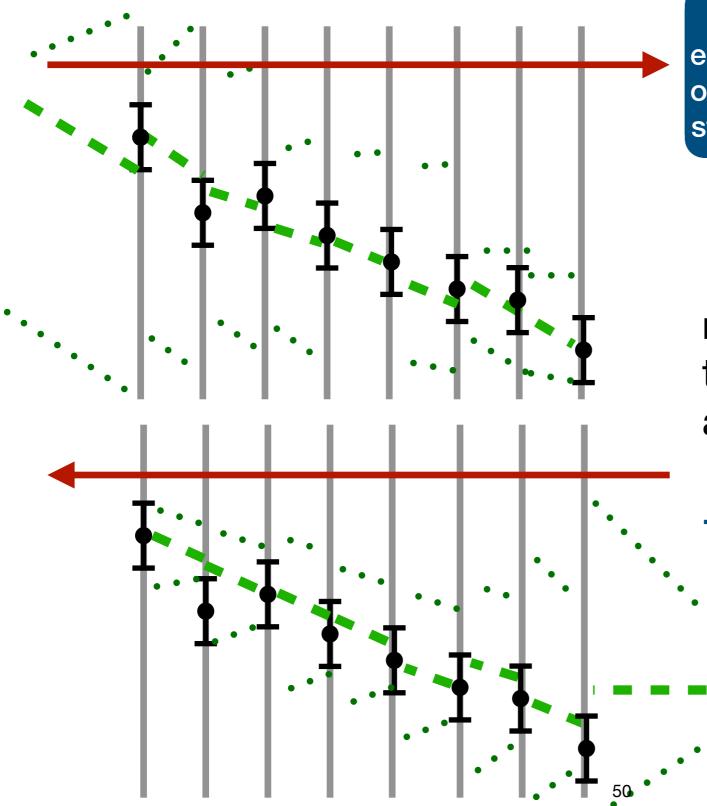
 $V_k \downarrow \Rightarrow K_k \uparrow \qquad \qquad C_k^{k-1} \downarrow \Rightarrow K_k \downarrow$

*if $dim(\alpha)$ is small you might use the weighted mean formalism instead of gain matrix formalism (faster): more in R.Fruwirth A. of K.F. to T. and V.F.



- there are no global parameters in Kalman filter
- the best track estimate is the last point

Smoother



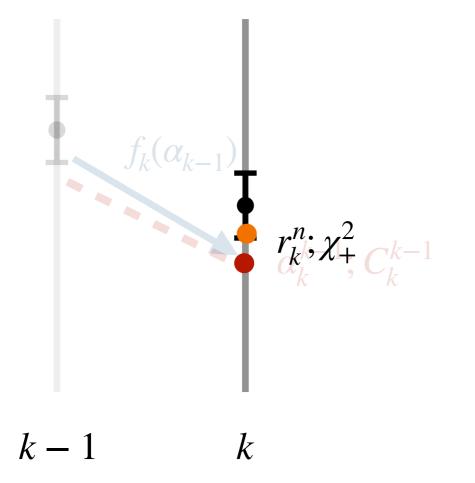
SMOOTHER

estimate precious track states based on everything known from the current state

run Kalman filter in reverse and take a weighted average at each plane

+ simpler math

Smoother



SMOOTHER

estimate precious track states based on everything known from the current state

alternative smoothing:

Goal: minimize χ^2_+

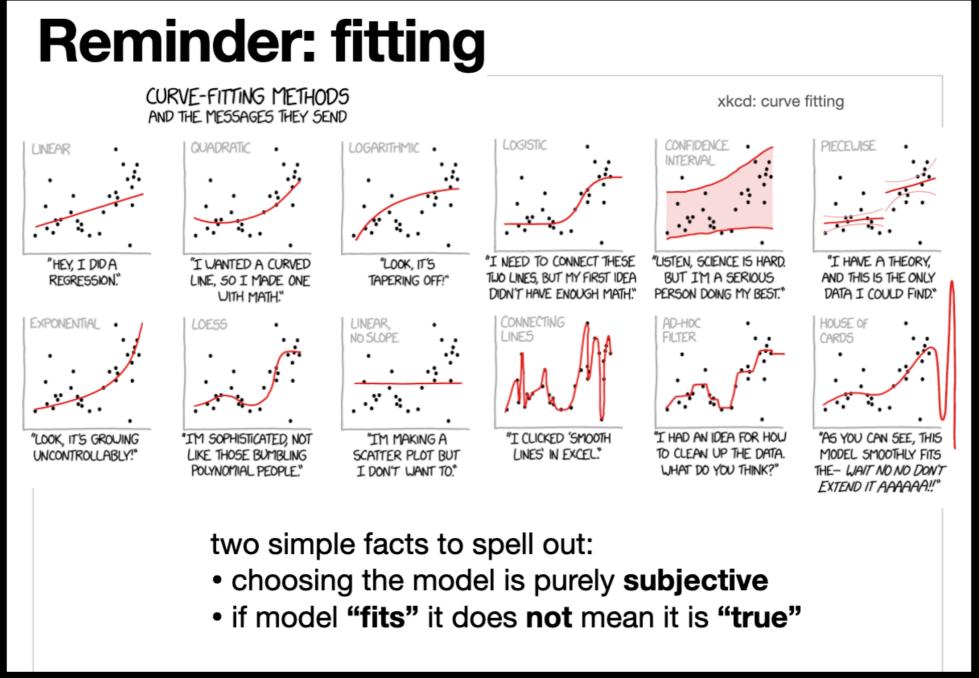
$$\alpha_{k-1}^{n} = \alpha_{k-1} + A_{k-1}(\alpha_{k}^{n} - \alpha_{k}^{k-1})$$

smoother gain matrix

weight of the prediction with information of all measurement versus current state

 α : track parameters

What is the track* we draw?

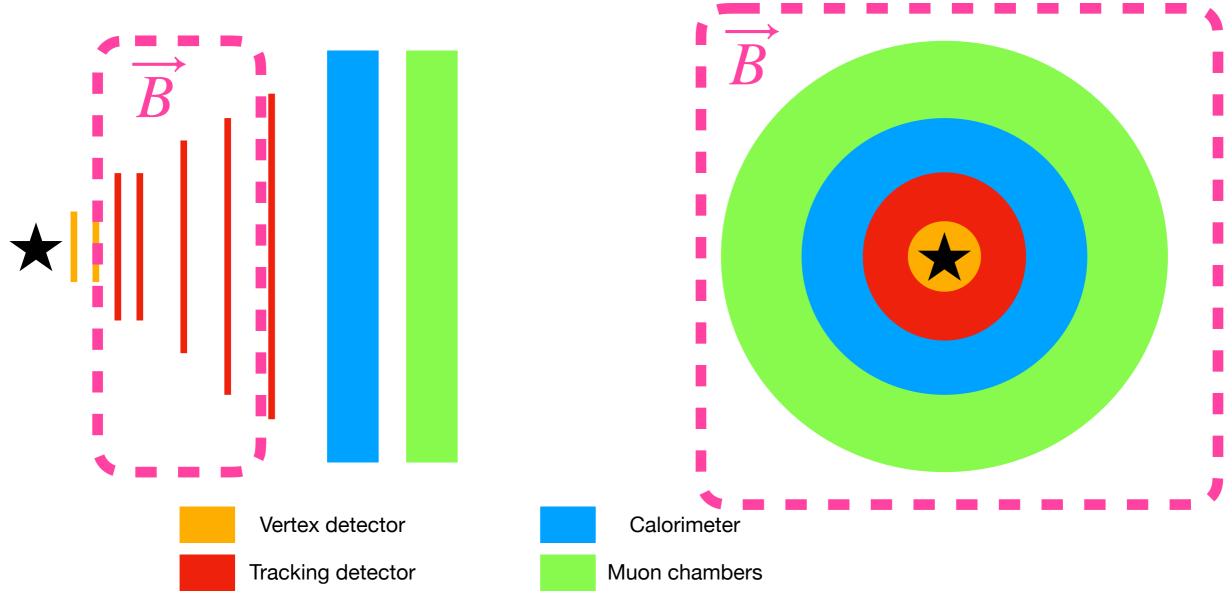


*What is α ?

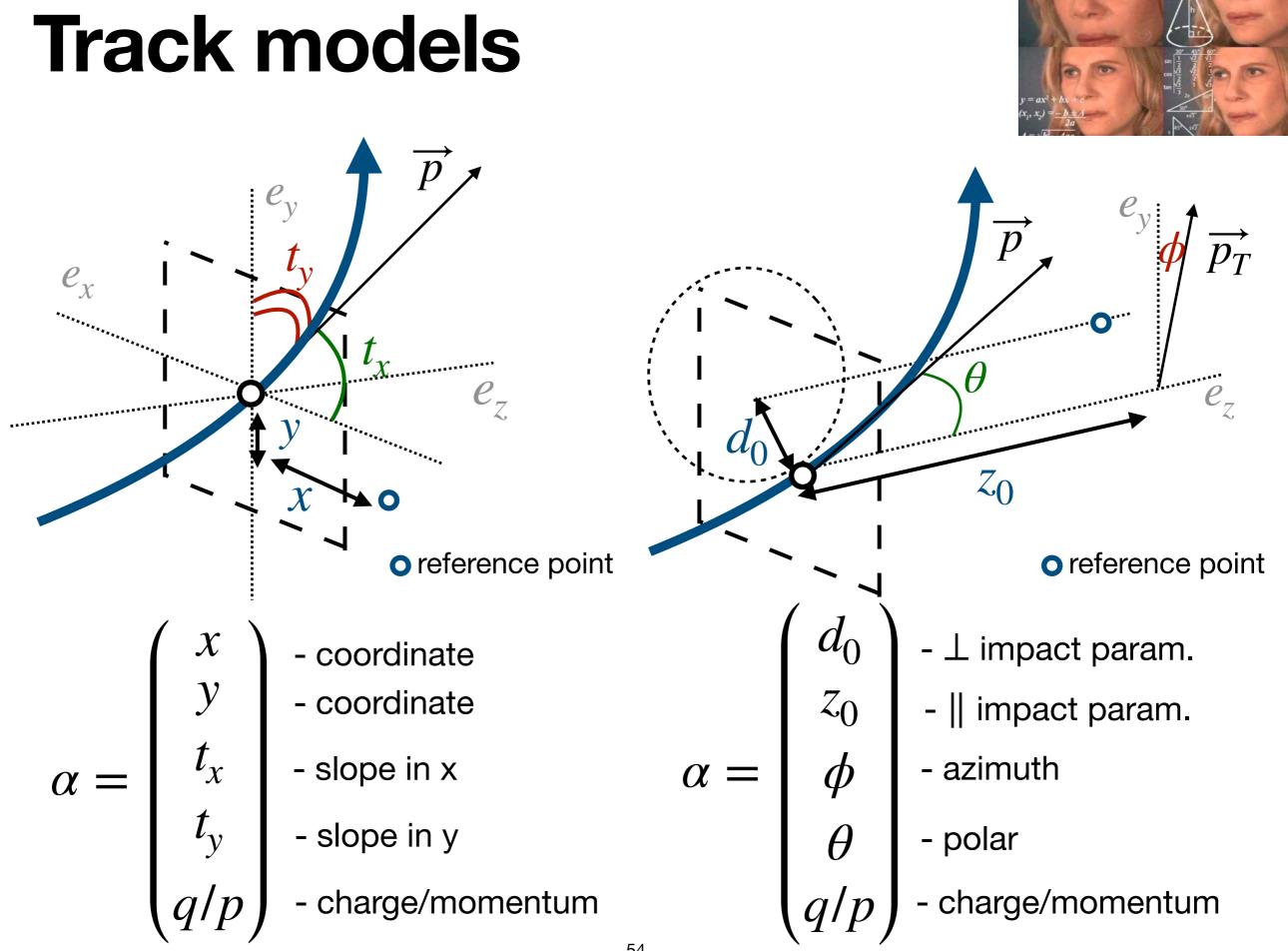
Track models

Detector geometry

• Forward



Collider

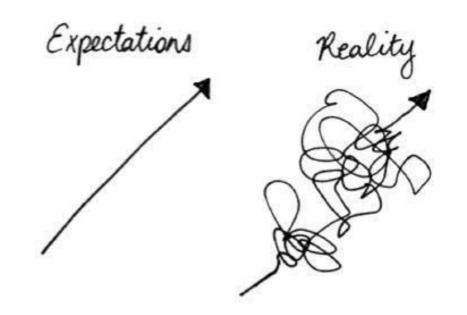


How good is my fitter? A check list

1. Check pulls of the input data:
$$p = \frac{x_i - x_{true}}{\sigma_i}$$

- 2. Check pull of the track parameters if you know "true" ones
- 3. Check hit residuals : $\hat{r}_i = m_i h_i(\hat{\alpha})$; $var(r) = V HCH^T$ and residual pull : $p = \frac{1}{\sqrt{var(r_i)}} \propto G(0,1)$

Track parameters correlate residuals!



Reality

- There is magnetic field/non-linear propagation
- There is noise
- There is energy loss
- Residual is not a point-to-point residual, based on the measurement technique and detector design
- One fit is often not good enough



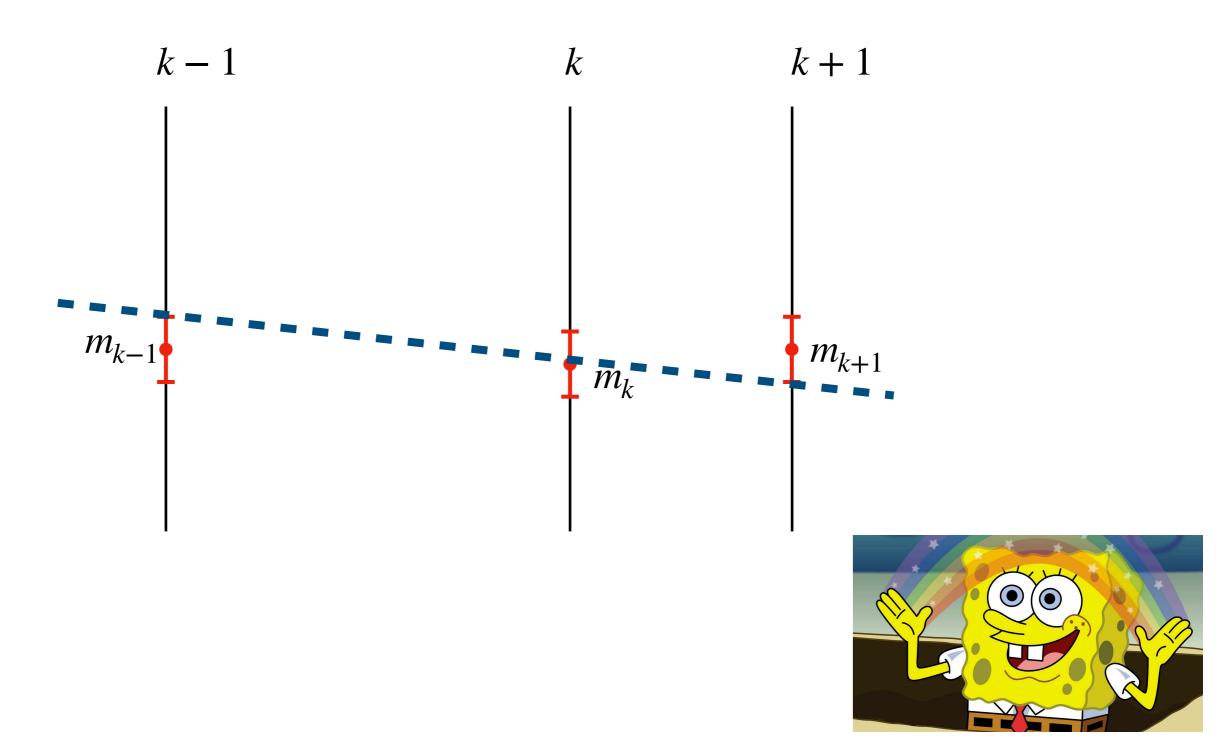


- There is magnetic field/non-linear propagation Taylor series
- There is noise inflate prediction uncertainty
- There is energy loss inflate prediction uncertainty
- Residual is not a point-to-point residual, based on the measurement technique and detector design - correct projection
- One fit is often not good enough multiple iterations



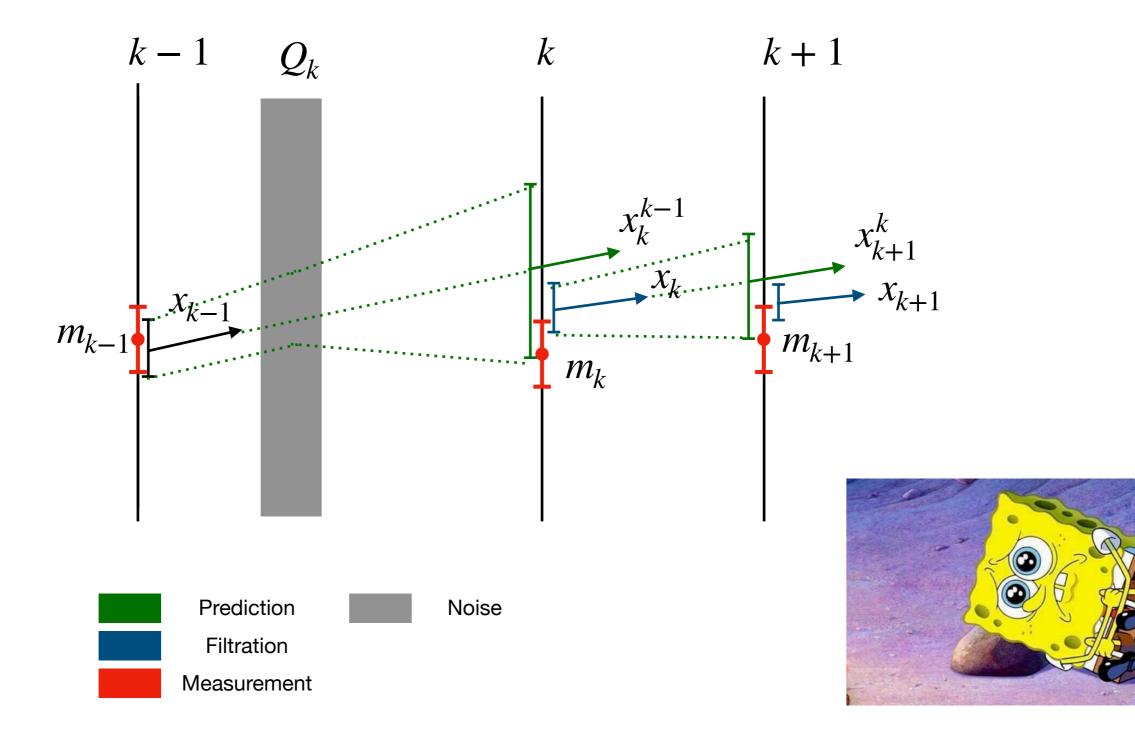
back on track... "second lecture"

Started with



Ended up with

Theoretically Kalman filter is an ideal fitter!



Kalman filter problems

Practical implementation Reality bites back

- 1. $K_k \propto (R_k^{k-1})^{-1}$: matrix inversion is expensive $\mathcal{O}(N^3)$ and unstable
- 2. Kalman filter is prone to numerical instabilities
- 3. Kalman filter is prone to outlier biases
- 4. Kalman filter assumes linearity and Gaussian errors
- 5. Kalman filter uses given assumption on the "zero"-state (initialisation)

Problem 1: Matrix inversion is still a pain

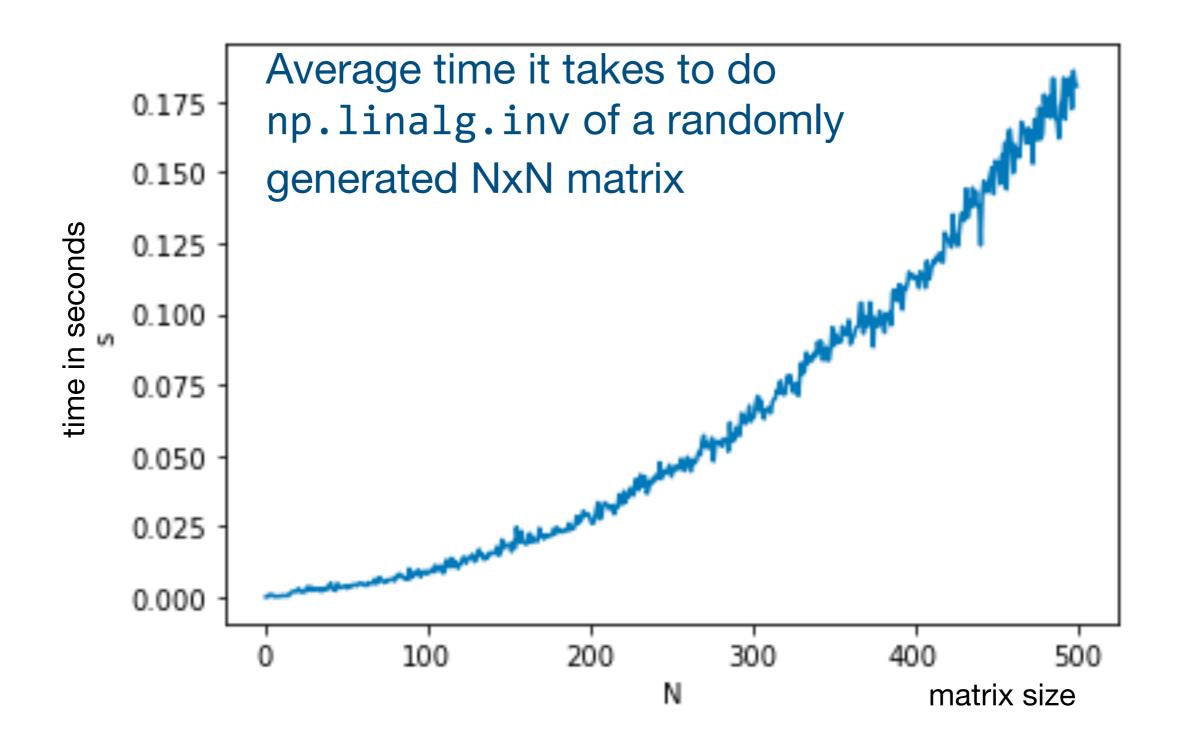
$$K_k = C_k^{k-1} H_k^T (R_k^{k-1})^{-1}$$
 and $\chi^2 \propto R_k^{-1}$

- 1. computationally expensive : $\mathcal{O}(N^3)$
- numerically unstable: prone to rounding errors especially bad for <u>ill-conditioned</u> matrices

For a typical tracking problem N = 5

 K_K - gain matrix C_k^{k-1} - predicted variance matrix after propagation H_k - projected propagation state derivative matrix R_k^{k-1} - residuals variance

Problem 1: Matrix inversion is still a pain



Problem 1: Matrix inversion is a pain Computational costs

• Still a fascinating problem for mathematics (even if the results might be of questionable practical use):

	Matrix inversion	One $n imes n$ matrix	One $n imes n$ matrix	Gauss-Jordan elimination	$O(n^3)$
				Strassen algorithm	$O(n^{2.807})$
				Coppersmith–Winograd algorithm	$O(n^{2.376})$
				Optimized CW-like algorithms	$O(n^{2.373})$

wikipedia

General truth: avoid inverting matrix at all costs See this great post

Part 1 : Catastrophic cancelation

$$C_k = (1 - K_k H_k) C_k^{k-1}$$

- $K_k H_k \approx 1 \Rightarrow$ "catastrophic cancellation"
- Often appears in the beginning of filter or when you encounter the first measurement that matters

Catastrophic cancellation example

$$a = 5.34587; b = 5.34585$$

Exact:
 $a^2 - b^2 = 28.5783260569 - 28.5781122225 = 0.0002138344$
Rounding:
 $a^2 - b^2 = 28.57833 - 28.57811 = 0.00022$

float: 7 decimal digits

double : 15 decimal digits

Part 1 : Catastrophic cancelation

$$C_k = (1 - K_k H_k) C_k^{k-1}$$

• $K_k H_k \approx 1 \Rightarrow$ "catastrophic cancellation"

Worse iteratively: example* evaluating $sin^2(\frac{\pi}{\Lambda})$

$$0.5 - 2^{-53}$$

 $0.5 - 2^{-52}$

iteration	χ^2	$\Delta \chi^2$	χ^2	$\Delta \chi^2$
1	2189.660 <mark>8022288765</mark>	2189.660 <mark>8022288765</mark>	2189.660 <mark>9616291444</mark>	2189.660 <mark>9616291444</mark>
2	2205. <mark>8925415651697</mark>	16.2317393363932131	2205.7475274721887	16.086565843044355
3	2204.1624495187029	1.7300920464667797	2203.8047379025147	1.9427895696740052
4	2203.3737431764907	0.78870634221220826	2204.010212472562	0.20547457004795433
5	2203.7285494796347	0.35480630314395967	2203. <mark>94089768533</mark>	0.069314787229814101
6	2203.812855194968	0.084305715333812259	-	-

*from S.Ponce

Part 2: Stability under $K + \delta K$

$$C_k = (1 - K_k H_k) C_k^{k-1}$$

- C_k must be posdef matrix otherwise not a valid covariance matrix
- C_k can become negdef
- And convergence for fitter is harder
- Many attempts to solve numerical instabilities: choosing correct constraints on the errors (especially first state errors), robust extended Kalman filter [G.A. Einicke, L.B. White], square root filter [P. Kaminski, A. Bryson, S.Schmidt]

Part 2 : Stability under $K + \delta K$

$$C_k = (1 - K_k H_k) C_k^{k-1}$$

 $K \to K + \delta K$

$$C_k^{new} = (1 - (K_k + \delta K)H_k)C_k^{k-1} = C_k - \delta K H_k C_k^{k-1}$$

Small deviations in gain matrix K might lead to negdef C_k



Part 2 : Stability under $K + \delta K$

$$C_{k} = (1 - K_{k}H_{k})C_{k}^{k-1}$$

$$C_{k} = (1 - K_{k}H_{k})C_{k}^{k-1}(1 - K_{k}H_{k})^{T} + K_{k}V_{k}K_{k}^{T}$$

This is just an error propagation of $\alpha_k = \alpha_k^{k-1} + K_k r_k^{k-1}$

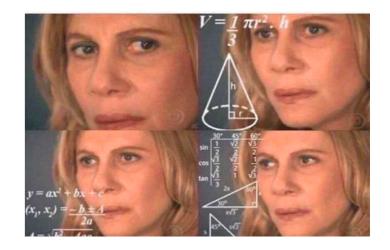


Part 2 : Stability under $K + \delta K$

$$C_k = (1 - K_k H_k) C_k^{k-1}$$

$$C_k = (1 - K_k H_k) C_k^{k-1} (1 - K_k H_k)^T + K_k V_k K_k^T$$





Problem 2: Numerical stability of Kalman filter

Part 2 : Stability under $K + \delta K$

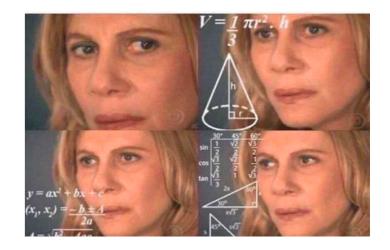
$$C_k = (1 - K_k H_k) C_k^{k-1}$$

$$N^3 + \mathcal{O}(N^2)$$

$$C_k = (1 - K_k H_k) C_k^{k-1} (1 - K_k H_k)^T + K_k V_k K_k^T$$

$$3N^3 + \mathcal{O}(N^2)$$





Problem 2: Numerical stability of Kalman filter

Part 2 : Stability under $K + \delta K$

$$C_{k} = (1 - K_{k}H_{k})C_{k}^{k-1} \qquad N^{3} + \mathcal{O}(N^{2})$$

$$C_{k} = (1 - K_{k}H_{k})C_{k}^{k-1}(1 - K_{k}H_{k})^{T} + K_{k}V_{k}K_{k}^{T} \qquad 3N^{3} + \mathcal{O}(N^{2})$$

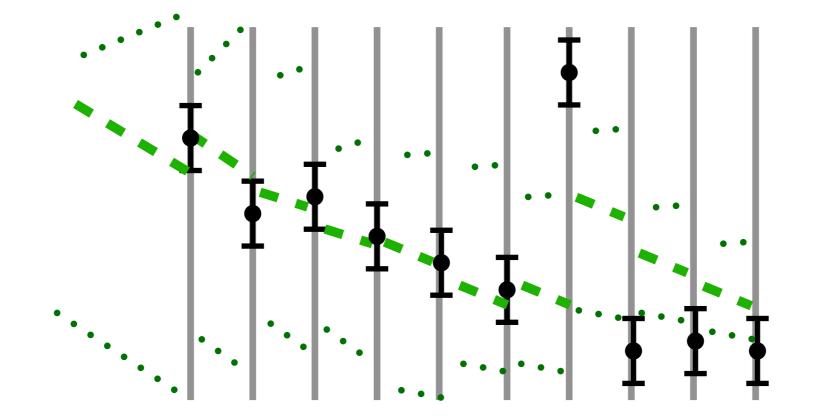
$$C_{k} = C_{k}^{k-1} - K_{k}(2H_{k}C_{k-1} - (V_{k} + H_{k}C_{k}^{k-1}H_{k}^{T})K_{k}^{T}) \qquad N^{3} + \mathcal{O}(N^{2})$$

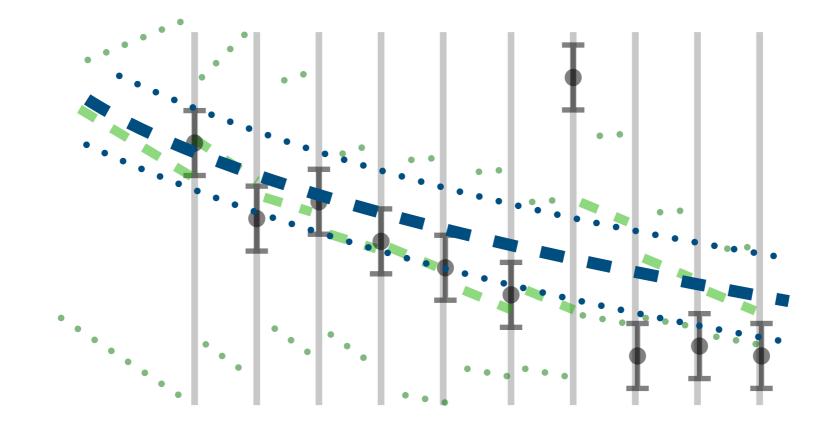


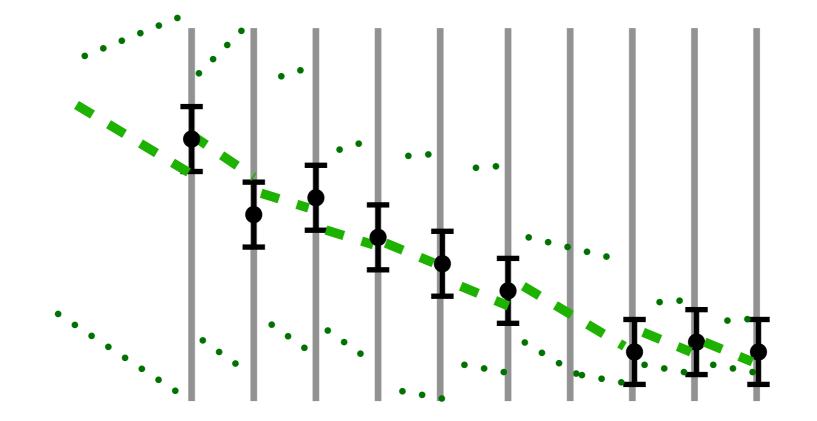
unstable \wedge stable against $K + \delta K$

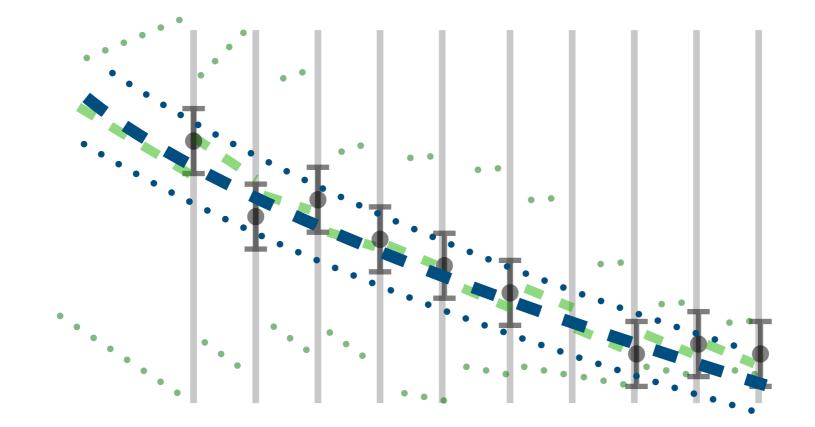


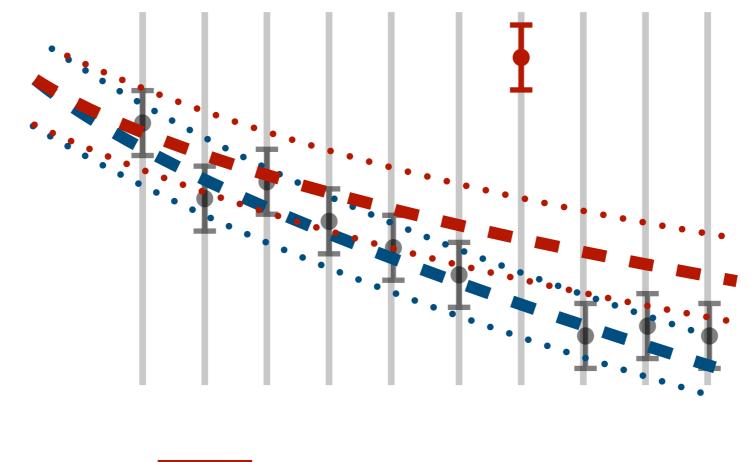
- Pattern recognition can make mistakes it is a wrong track
- It can be an unfortunate event see δ -rays for example
- Can be electronics noise (if it is often the case in LHCb VELO, you can safely blame me)

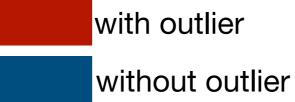






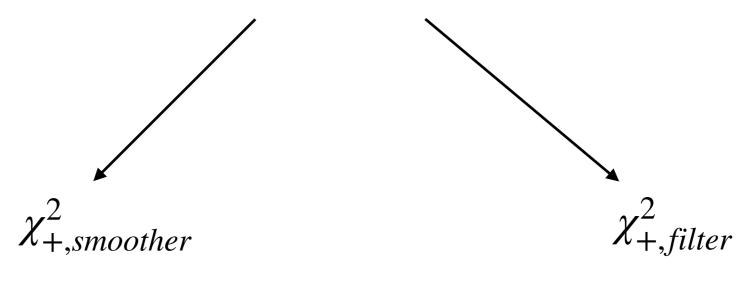






Solution: χ^2_+

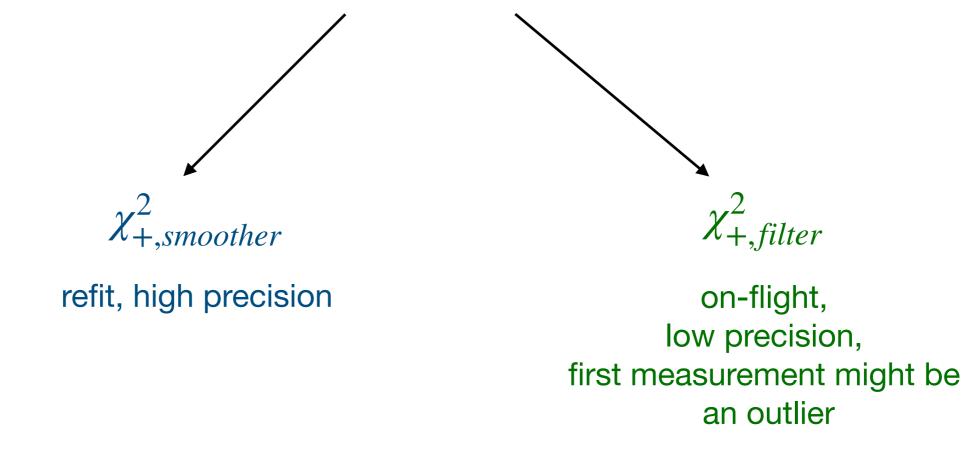
• If χ^2_+ is too big, reject the measurement



Which χ^2_+ is better to use?

Solution: χ^2_+

• If χ^2_+ is too big, reject the measurement



Can you already spot a problem with any outlier removal?

Outlier removal increases hit purity but decreases hit efficiency

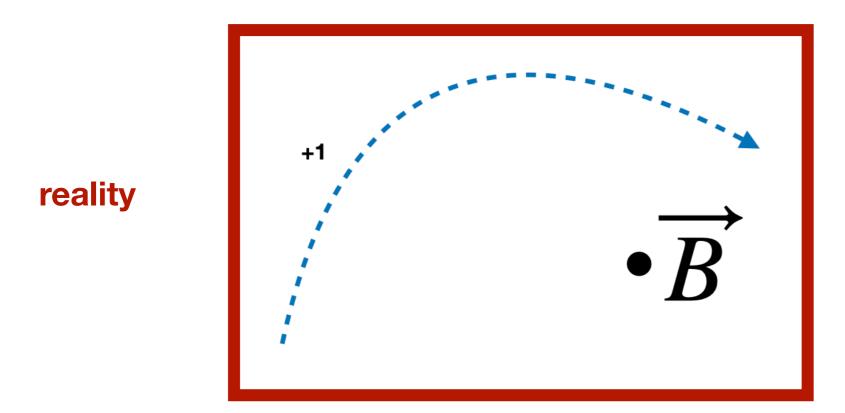
Hit purity: fraction of correct hits per track Hit efficiency: fraction of all correct hits found

This is by no means the entire story - there are advanced outlier removal techniques and outlier-robust Kalman filters [E. Chabanat, N. Estre], [G.Agamennoni, J.I. Nieto, E.M. Nebot]

Problem 4: Kalman filter assumptions

Part 1: linear propagation

 Basic assumption of Kalman filter - linear model for propagation, but



Taylor expansion around reference state

Problem 4: Kalman filter assumptions

Part 2: non-Gaussian errors

- Another assumption of Kalman filter Gaussian errors
- In reality:
 - Non-gausian noise
 - Non-gaussian energy loss
 - Non-gaussian scattering

Especially important for electrons in material heavy detectors, like ATLAS or CMS

Problem 4: Kalman filter assumptions Part 2: non-Gaussian errors - Gaussian Sum Filter

 Replace non-gaussian effect by a weighted sum of gaussians gaussian sum filter

filtered state:
$$G(\alpha_k, C_k) \Rightarrow \sum_{i=0}^{L} b_i G(\alpha_k^i, C_k^i)$$

 b_L - weights, L - number of the Gaussian components

Problem 4: Kalman filter assumptions Part 2: non-Gaussian errors - Gaussian Sum Filter

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Problem:

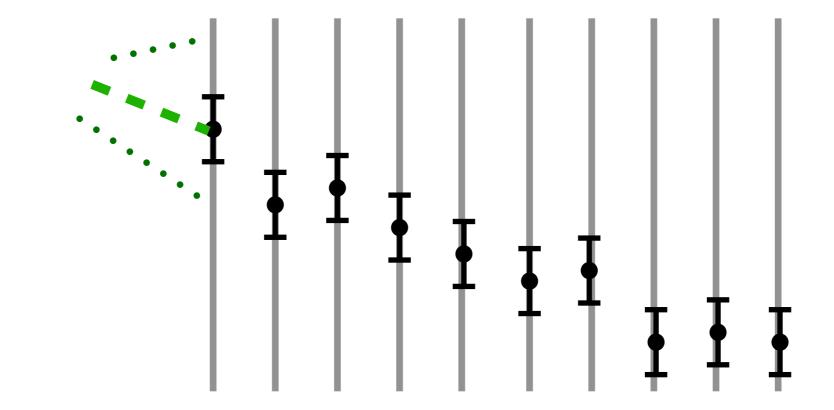
• L filtrated states per measurement - computations complexity increases as L^k

Solutions:

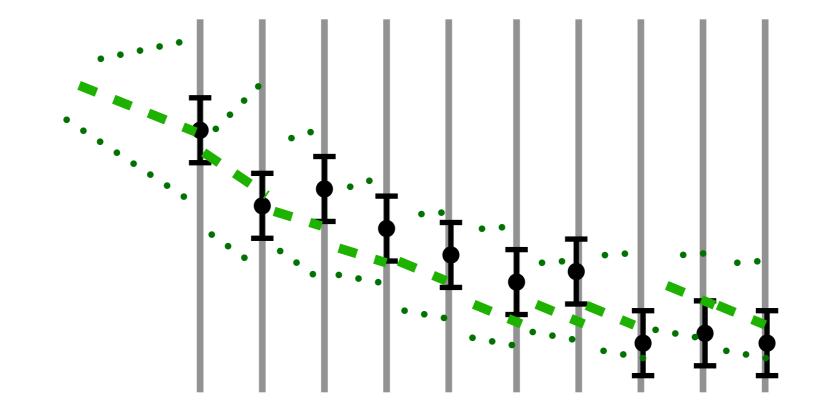
- ignore low-weight Gaussians
- merge Gaussians based on similarity (see Kullback-Leiber distance)

• Kalman filter is a recursive algorithm : has to know state 0

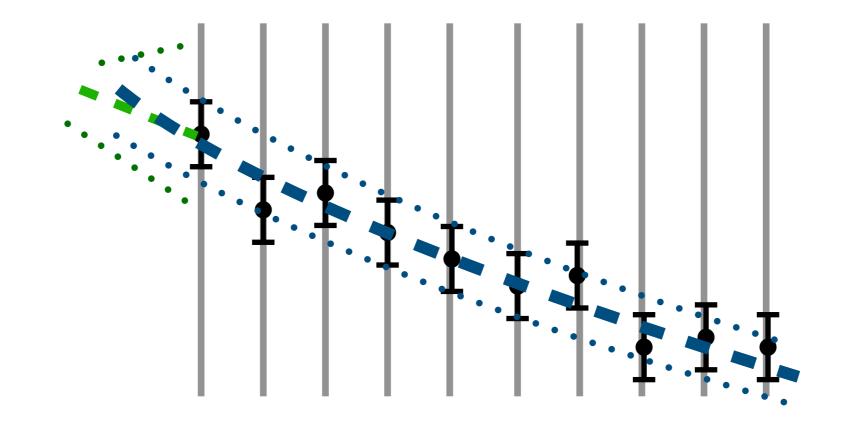
- Kalman filter is a recursive algorithm : has to know state 0
- Good first guess



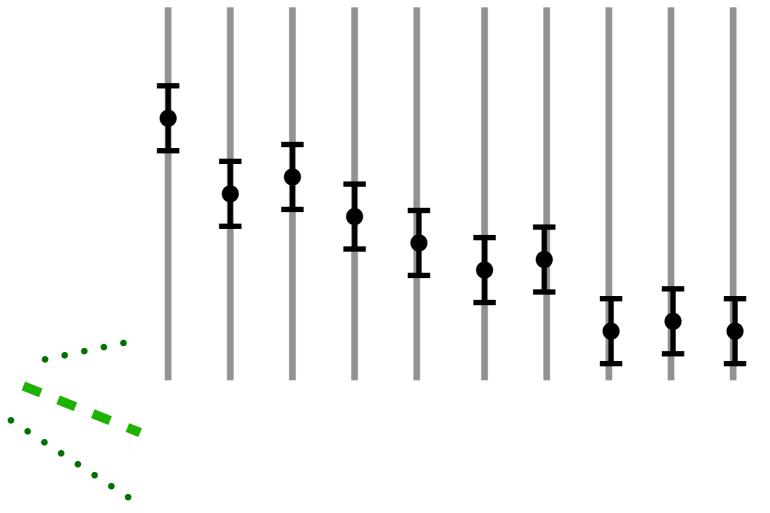
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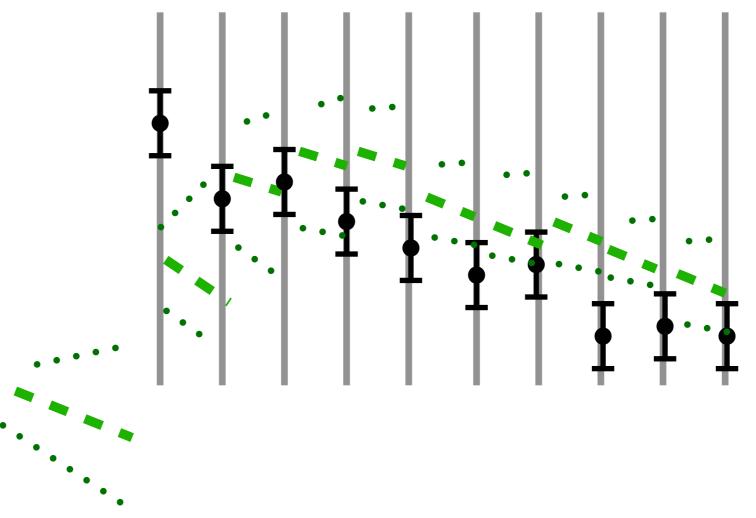
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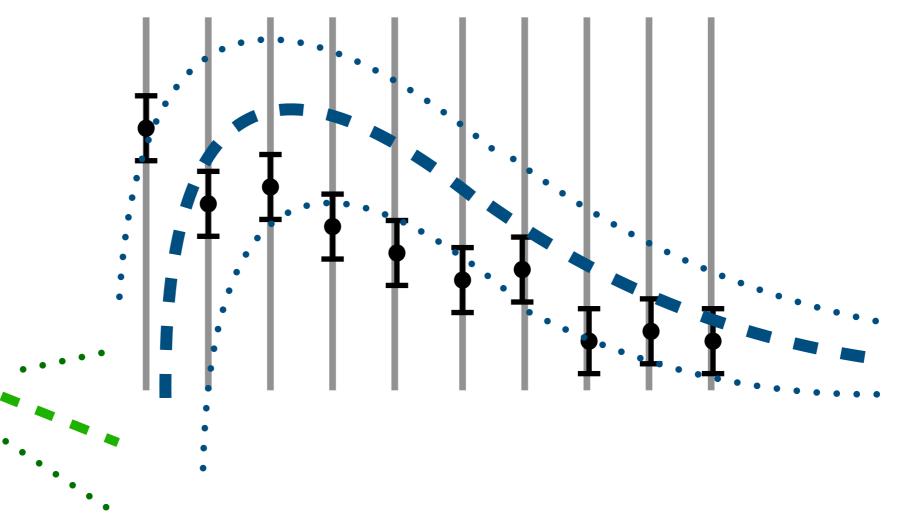
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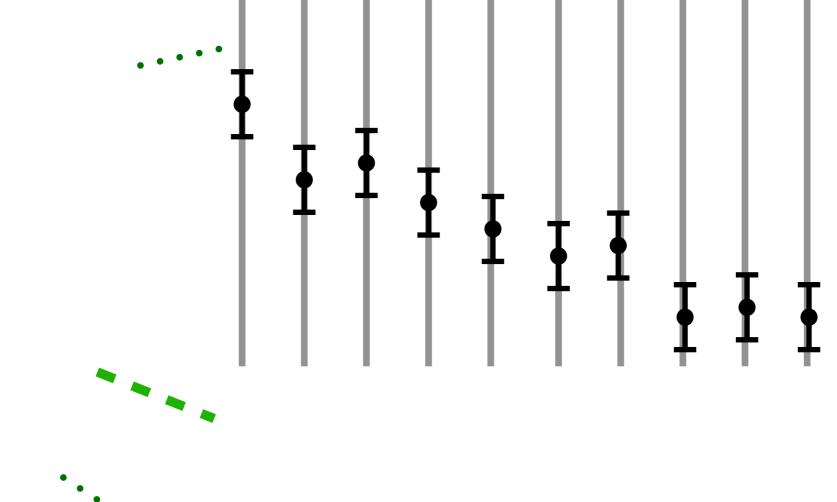
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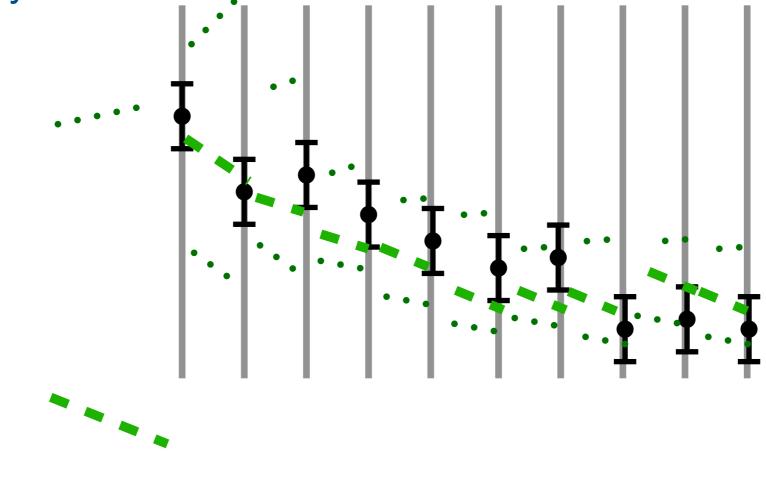
- Kalman filter is a recursive algorithm : has to know state 0
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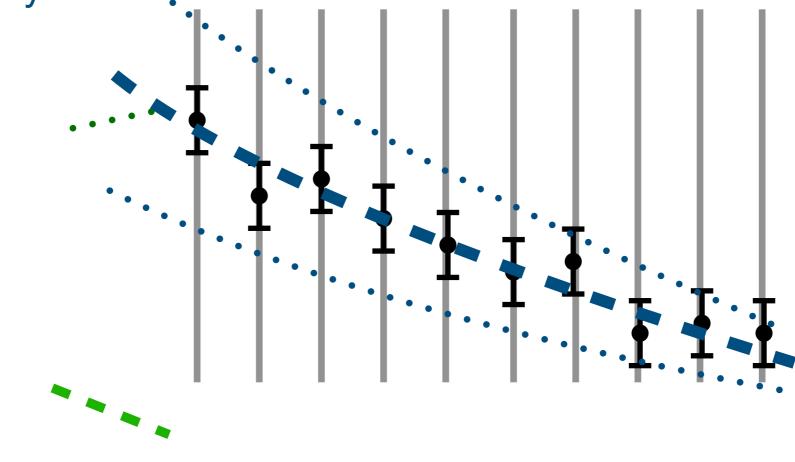
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 .



- Kalman filter is a recursive algorithm : has to know state 0
- Bad first guess but acknowledging it is bad : assign bigger uncertainty BUT not TOO big uncertainty \rightarrow catastrophic cancellation in $C_k = (1 - K_k H_k) C_k^{k-1}$

More things to keep in mind



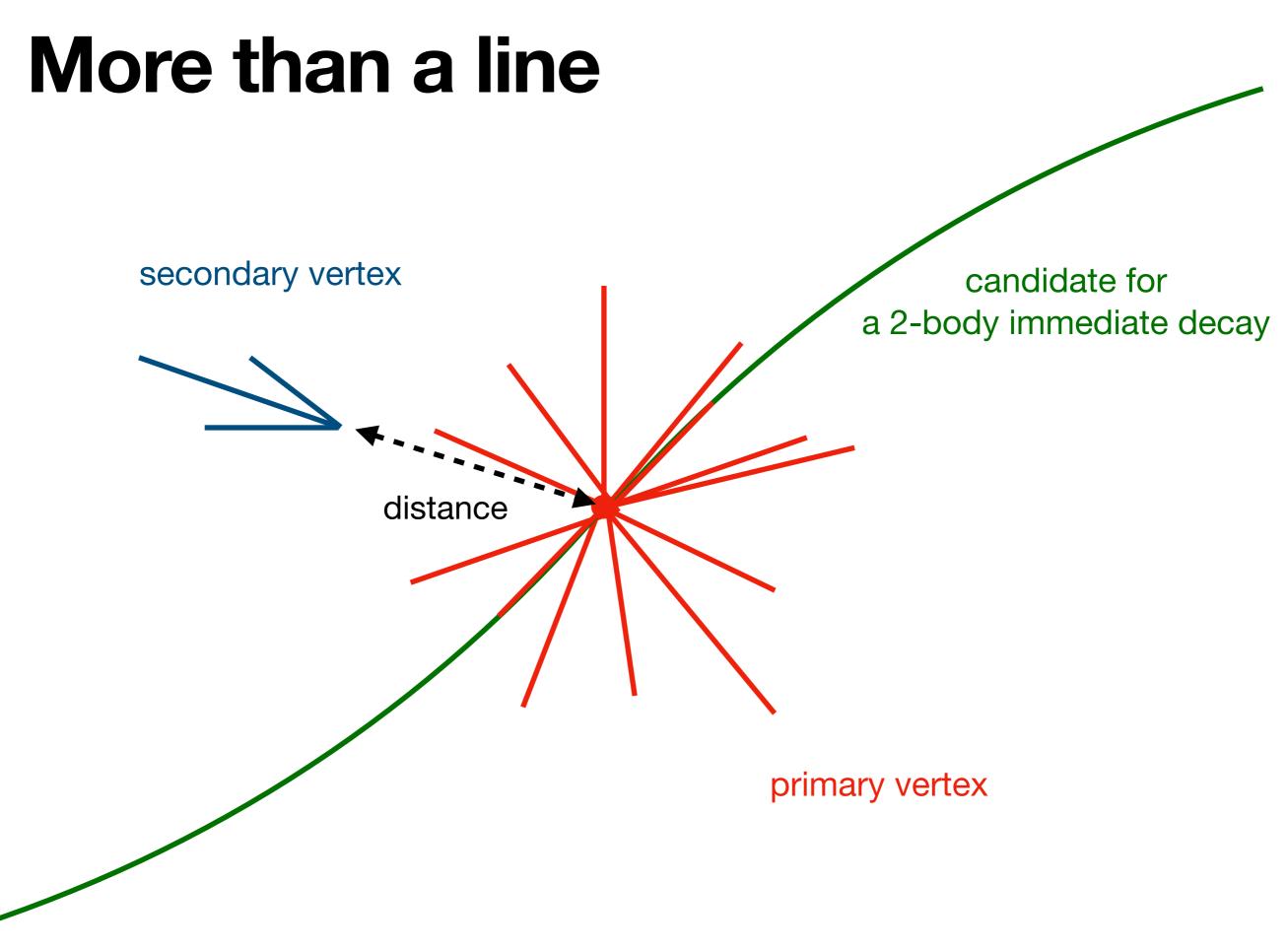
Detector aging Everything gets older

• irradiation over years leads to worse detector performance



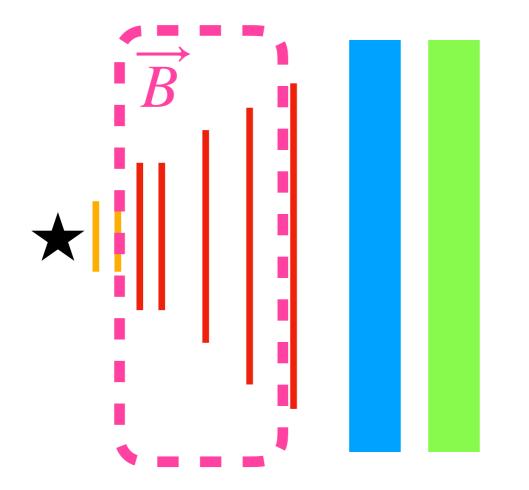
What you should make sure happens:

- continuous performance checks
- there is an easy way to change filter hardcoded conditions, like outliers removal χ^2

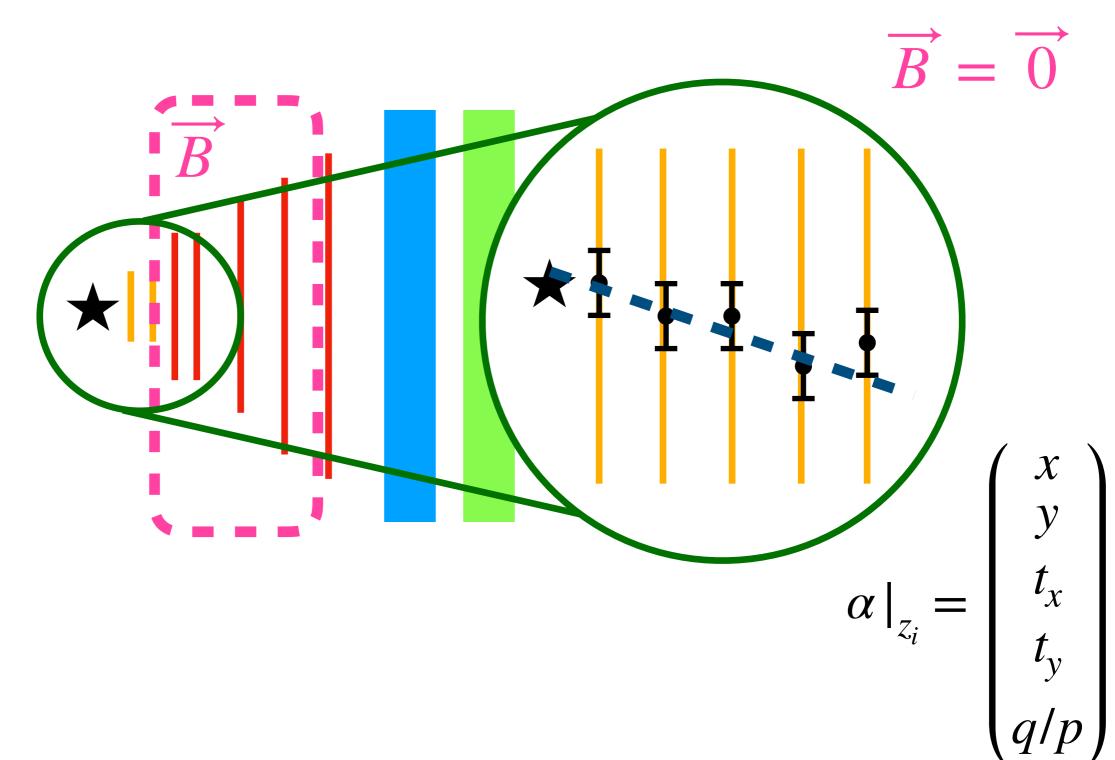


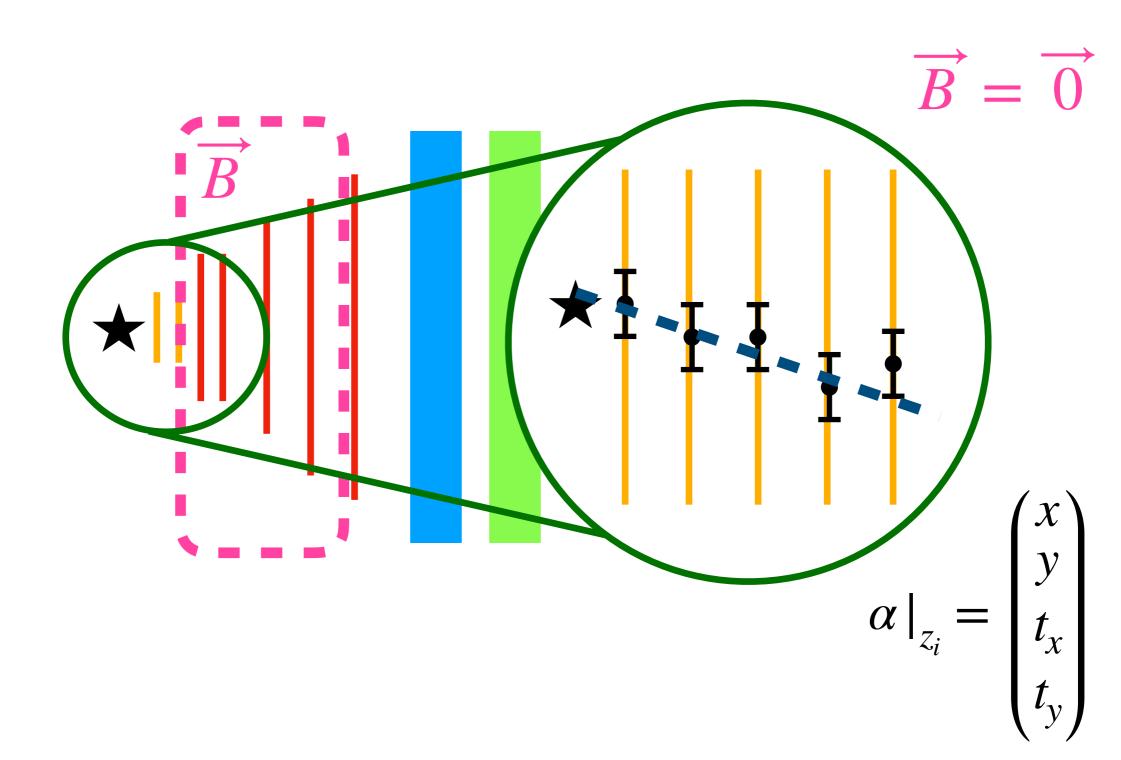
Can I cheat?

A simple LHCb-like example

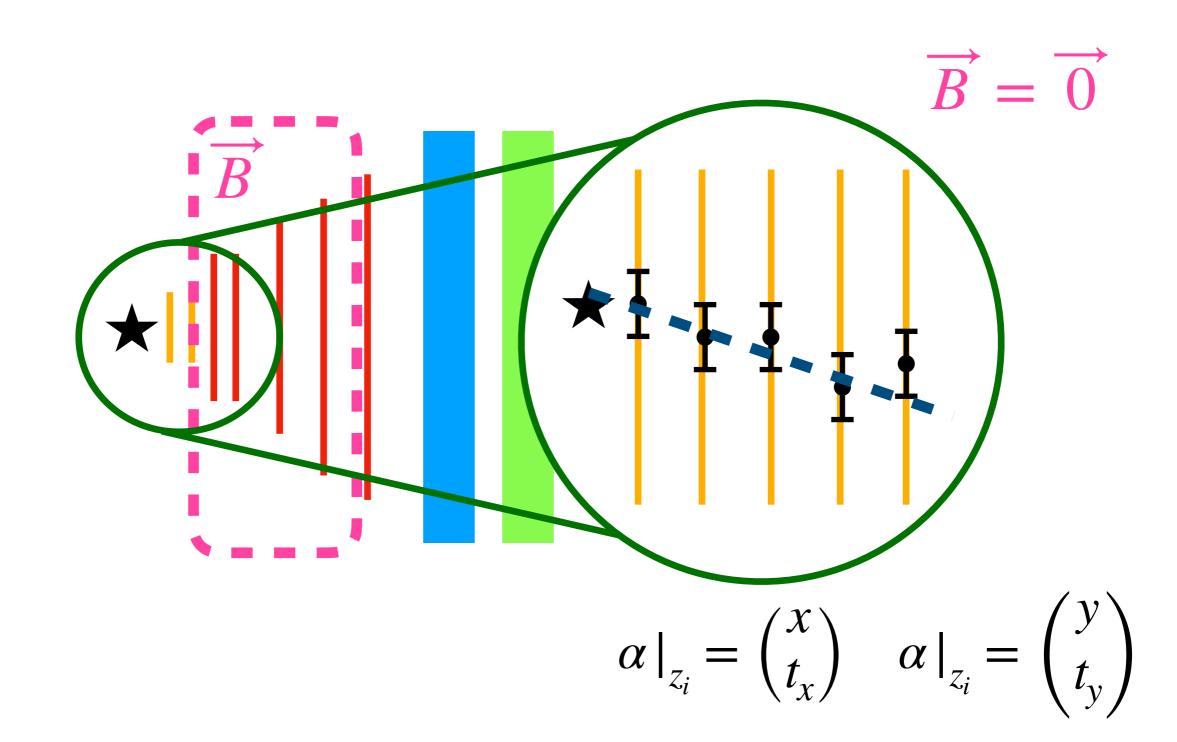


$\vec{B} = \vec{0}$





q/p is not required in the computation but might still be associated to the track from the track finding algorithm



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Parallelisation

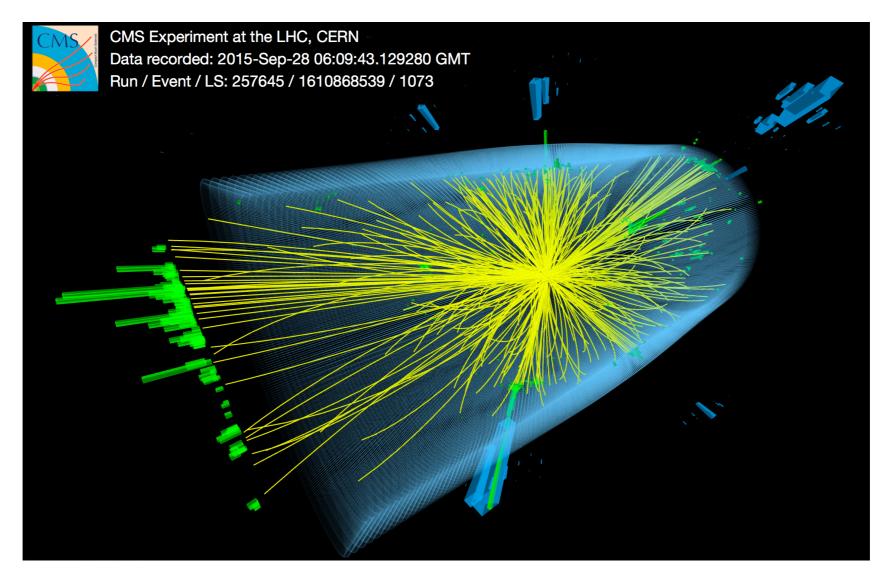


Simply parallelizable?



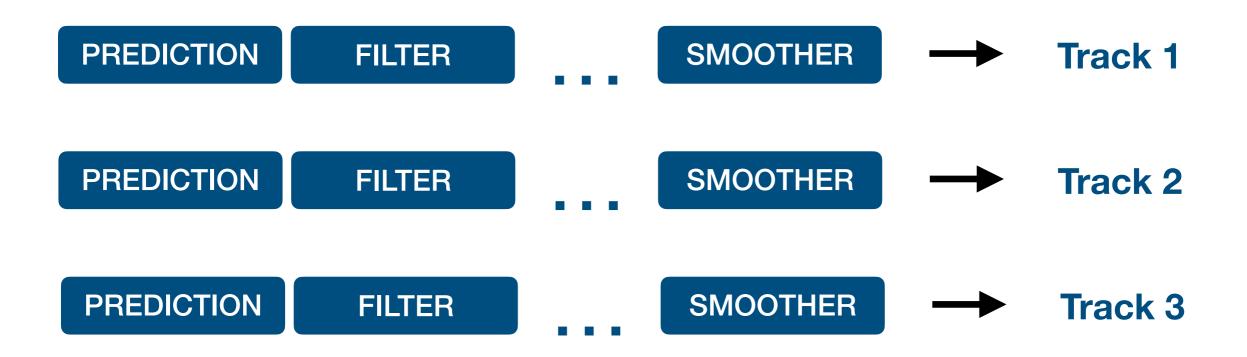
Simply parallelizable?





But in reality you have hundreds of tracks

Simply parallelizable?

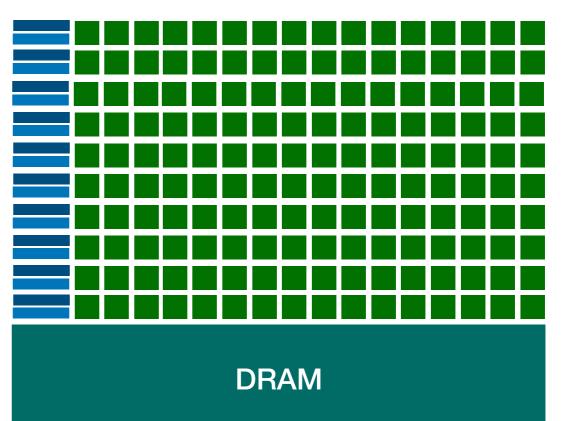




CPU vs GPU

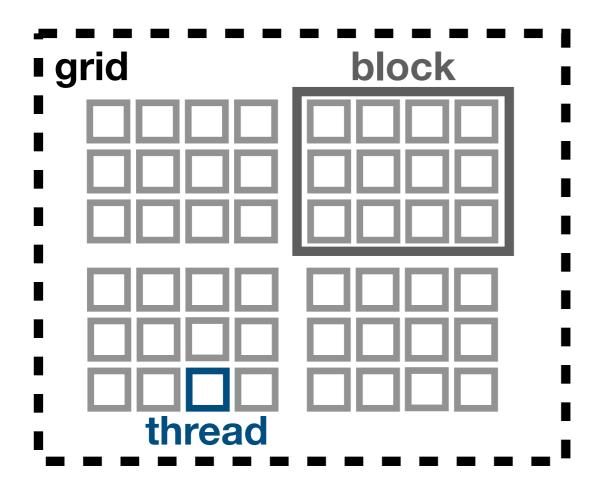
CPUalualucontrolalualualucacheDRAM



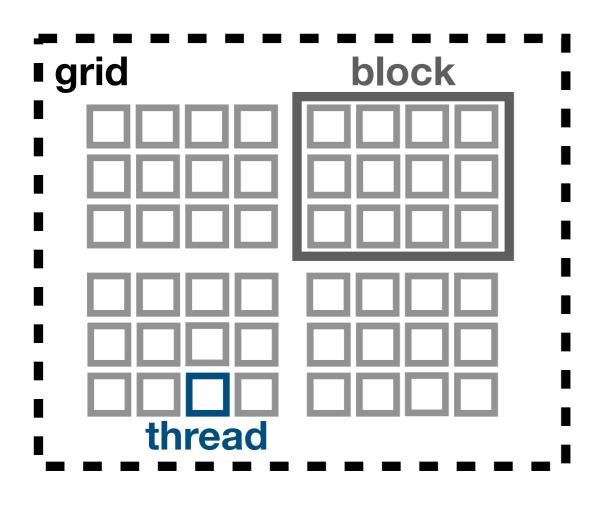


- Serial-oriented
- Low-latency
- Fewer cores, but powerful
- SIMD

- Parallel-oriented
- High-latency
- More cores, but less powerful
- SIMT



- each block of threads has shared memory
- two parallelisations
 - track level : each thread is a track
 - intra-track : each block is a track,
 - each thread is a parallelised operation



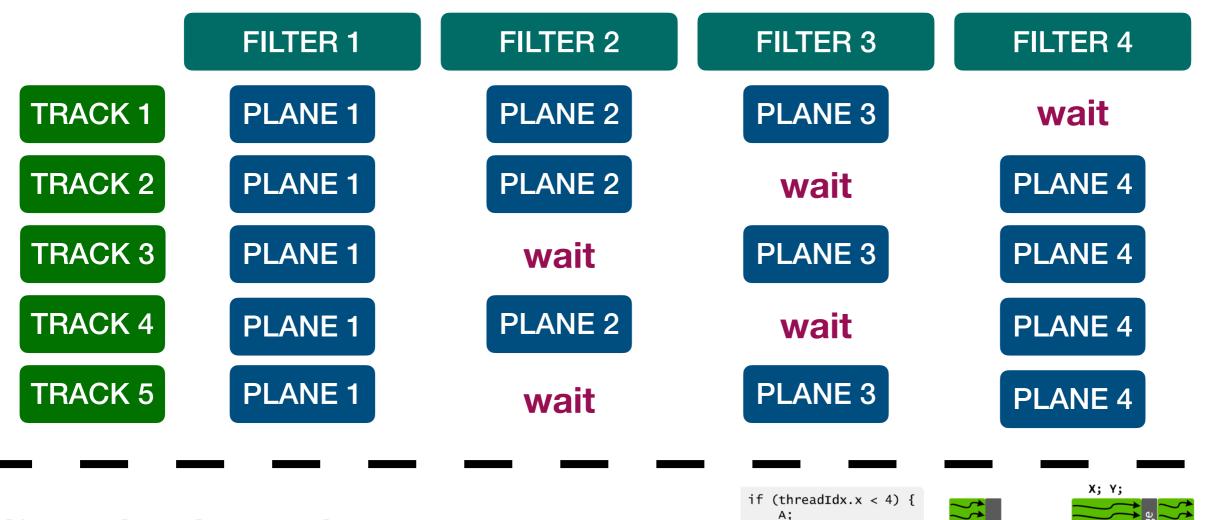
- each block of threads has shared memory
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 - track level : each thread is a track
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 - each thread is a parallelised operation

Problems with GPU

- 1. Handling code divergence
- 2. Limited memory
- 3. Slow transfer of data to/from GPU

Problem 1 : command divergence

 Single Instruction Multiple Thread : assumes commands are the same for all tracks, if not - inefficiency



if-else blocks are dangerous for the same reason (branch divergence):

Note: on modern GPUs there are ways to improve on divergence

B; } else { X:

Υ;

A; B;

Z;

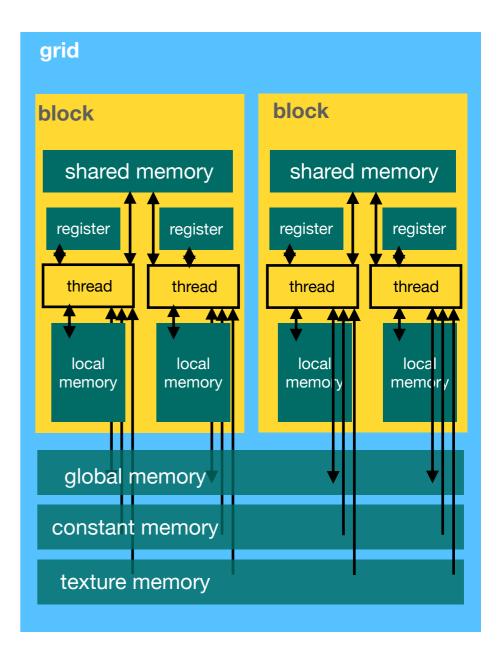
Time

}

Z;

Problem 2 : limited memory

- Limited memory per thread : especially problematic for recursive functions
- Numeric precision and rounding is typically worse



Problem 2 : limited memory

- Limited memory per thread : especially problematic for recursive functions
- Numeric precision and rounding is typically worse

size small big register texture constant shared and local global $\mathcal{O}(0.1kB)$ $\mathcal{O}(kB)$ 64kB $\mathcal{O}(10-100kB)$ $\mathcal{O}(GB)$

grid grid block block shared memory shared memory register register register register thread thread thread thread local local local local memory memory memory memory global memory global memory constant memory constant memory texture memory texture memory

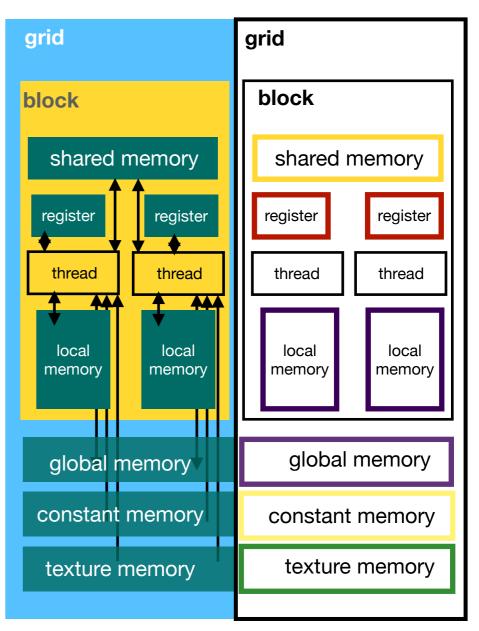
Note: this is all approximate as concrete numbers depend on the card, but gives you a rough idea of orders

memory

Problem 2 : limited memory

- Limited memory per thread : especially problematic for recursive functions
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big small size register texture constant shared and local global $\mathcal{O}(GB)$ $\mathcal{O}(0.1kB) \quad \mathcal{O}(kB)$ 64kBO(10 - 100kB)fast slow access global and local texture constant register shared 300-800 50-100 1-3 1-3 0.5-1 clock cycles clock cycles clock cycles clock cycles access



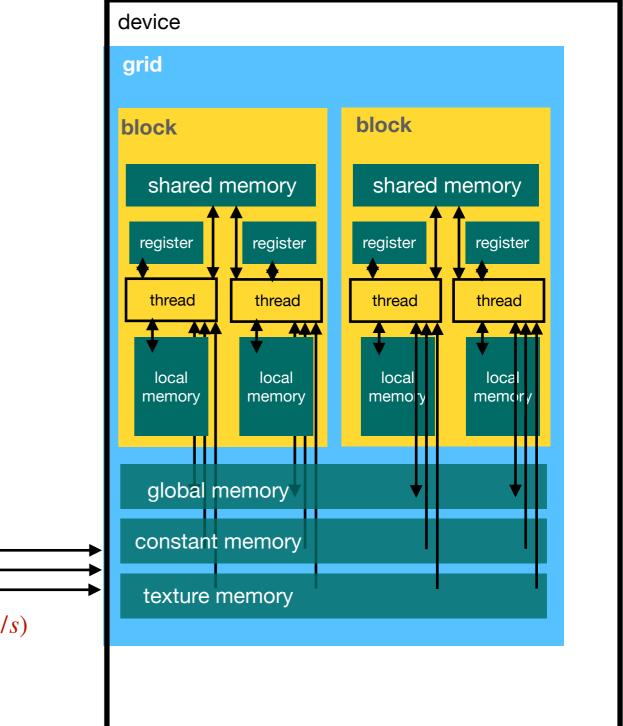
Note: this is all approximate as concrete numbers depend on the card, but gives you a rough idea of orders

Problem 3 : costly transfer

 Upload/download from/to GPU is slow - can take 1000s clock cycles

minimize host-device data transfer! host $\mathcal{O}(10GB/s)$

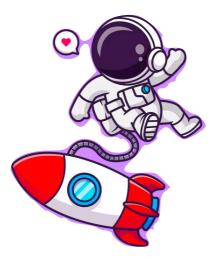






Big ideas to take home

- 1. Kalman filter is a powerful fitting tool : problem is simplified to 1-equations solving for M-times
- 2. Kalman filter implementation is tricky: numerical instabilities, outliers, initialisation, non-linearity etc.
- 3. Track fitting is a **good candidate for parallelisation**



The end?

