many measurements

$$M \approx Q^T \Sigma^{-1} Q$$

sensitivity

covariance of measurements

for HFC/IC with only pressure measurements, assume

$$\Sigma = I \sigma^2$$

identity

measurement covariance

simplification

$$M \approx Q^T (I \sigma^2)^{-1} Q$$

$$\approx Q^T (I \sigma^{-2}) Q$$

$$\approx \sigma^{-2} Q^T Q$$

for our pressure measurement, HFC/IC example

σ^2 : MPa^2 $\qquad$ σ^{-2} : MPa^{-2}

Q : $\dfrac{MPa}{\text{parameter units}}$

what are the units of M?

$$M \approx \sigma^{-2} \cdot Q^T Q$$

MPa^{-2} $\quad$ $\frac{MPa}{param}$ $\quad$ $\frac{MPa}{param}$

$param_i^{-1} \cdot param_j^{-1}$

$$\Sigma_\theta \approx M^{-1}$$

$param_i \cdot param_j$

Why did changing pressure from Pa to bar (or MPa) change the FIM?

suspect accidentally assumed $\underline{\sigma^{-2} = 1}$

Take away: changing measurement units does NOT change FIM

How to improve FIM scaling? Only choice is to scale θ.

How to scale θ?

↳ change units (possible changing Pa to bar changed units of θ)

→ To avoid this, one possible option is to scale all of the measurements for regression to be dimensionless

original regression model

$$P_j = f(x_j, T_j, \theta)$$

output has units

$$P_j = P_{ref} \cdot f(x_j, T_j, \theta)$$

output is dimensionless

↳ scale θ by the average value for FIM calculation

↳ log transform θ (only really do this for models that require an order of magnitude change)

regressing $k_{i,j} = f(T_j, \theta)$

dimensionless

check code

$$\boxed{\beta_1 \left(\frac{T_j}{T_{ref}}\right) + \beta_2 \left(\frac{T_j}{T_{ref}}\right)^2}$$

TODO: Bridgette check θ (or β) are dimensions

TODO: Jialu check assumed σ^2 in FIM calculation, update FIM calculation for 1 case, post to GitHub, agree, update everything

Question: does scaling objective in regression problem impact FIM estimate?

↳ if using parmest... for covariance matrix/FIM yes! Parmest gets the reduced Hessian of the opt. problem

↳ if using Pyomo.DoE... no! Pyomo.DoE gets Q directly from the model

TODO: Estimate σ^2 from data

$$\hat{\sigma}^2 = \frac{r^T \cdot r}{n - p}$$

$\vec{r}$: residuals vector
n: number of data points
p: number of fitted parameters

For each case study, what is $\hat{\sigma}^2$?

Hypothetical: 1000 Pa to 5000 Pa consistently across models

↳ perhaps agree on 3000 Pa

What is $\hat{\sigma}^2$ for the best fitting model for each system? TODO: Bridgette

Time line:

1. Bridgette verifies β is dimensionless
2. " computes $\hat{\sigma}^{-2}$ for all systems (best model), chooses number of $\hat{\sigma}^2$ to use for all FIM calcs
   one
3. Jialu computes FIM, also double check all scaling options are consistent with math posts to GitHub, gets feedback on order of magnitude for new D-, A, E-opt and eigen decomposition
4. Jialu recomputes FIM for all cases