INL/MIS-24-78470-Revision-0

# Bayesian Framework for Bioburden Density Estimation in Planetary Protection

June 2024

Changing the World's Energy Future

Mike DiNicola, Lisa Guan, Andrei Vasilyevich Gribok

Idaho National Laboratory

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**Idaho National Laboratory**
**Idaho Falls, Idaho 83415**

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Idaho National Laboratory

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California Institute of Technology

# *Bayesian Framework for Bioburden Density Estimation in Planetary Protection*

**Andrei Gribok[a], Lisa Guan[b], and Mike DiNicola[b]**

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# Goals and Objectives

- The current PP bioburden accounting workflow has many elements that can benefit from statistics/modeling-based methods
- Using a Bayesian Framework for bioburden estimation improves upon the current method via the following features:
  - Has a way to treat zero CFU measurements
  - Provides credible intervals for bioburden density estimate
  - Provides flexibility in reporting statistics (summary statistics of posterior distribution, credible intervals, or posterior distribution)
- The tool should provide a measure of accuracy (risk) for bioburden density estimation
  - Calculate Bayesian/frequentist risk for an estimator
- The tool needs to integrate the sampling efficiency model into its calculations
- The tool should handle specified and implied components
  - The specified and implied components are no data estimators

**Main objective is to develop a tool that can provide information on what the bioburden density is and how certain are we of it.**

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# Presentation Outline

1. Available data
2. Bayesian modeling and bioburden density estimation
3. Non-informative and informative priors
4. Bayesian approach as shrinkage
5. Risks of the estimators
6. Sampling efficiency as Poisson process thinning
7. Sampling optimization
8. Machine learning-informed approach to bioburden density estimation
9. Hierarchical Bayes

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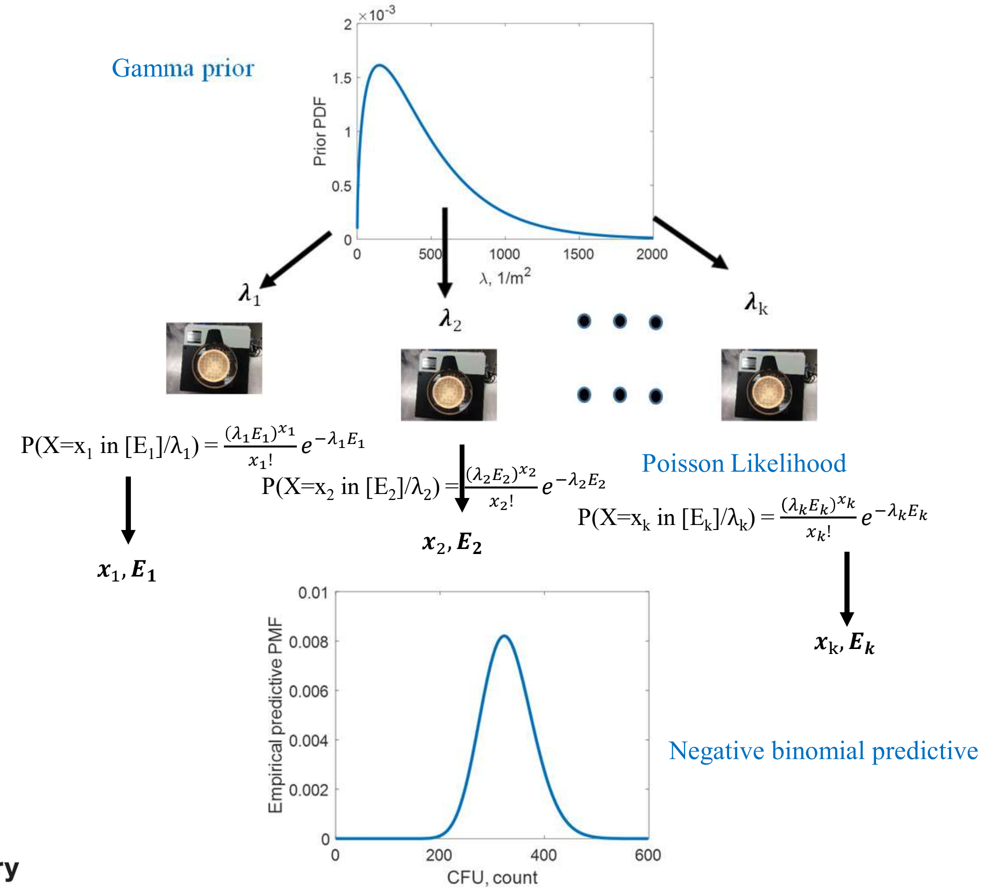
# Gamma-Poisson Bioburden Compound Distribution Model

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# Data Generating Model and Parameter Estimators

$X_i = x|\lambda_{true}^i \sim Poisson(\lambda_{true}^i \cdot E_i)$

$\lambda_{true}^i|\alpha,\beta \sim Gamma(\alpha,\beta), i = 1,\ldots N$

$\widehat{\lambda_i}(x_i) = \frac{x_i}{E_i}$ – Maximum Likelihood Estimator (MLE)

$\widehat{\lambda_i}(x_i) = \frac{x_i+\alpha}{E_i+\beta}$ – Conjugate prior Bayes Estimator

$\widehat{\lambda_i} = d$ – Deterministic Estimator

$X_i$ – random variable describing the number of CFUs on i-th sampled component
$x_i$ – observed number of CFUs in a sample from i-th sampled component
$E_i$ – exposure for a sample, determined by multiplying the sampled area by pour fraction
$\lambda_{true}^i$ – true bioburden density for a sample
$Gamma(\lambda/\ \alpha,\beta)$ – Gamma prior distribution of bioburden density $\lambda_{true}^i$
α,β – parameters of the Gamma prior distribution
$Poisson(\lambda_{true}^i \cdot E_i)$ – Poisson likelihood of having x CFU counts at exposure $E_i$ given $\lambda_{true}^i$
N – number of components/samples

| Component 261 Sample No. | CFUs Observed | Area Sampled, $m^2$ | Pour Fraction | Exposure, $m^2$ |
|---|---|---|---|---|
| 1 | 1 | 0.0025 | 0.8 | 0.0020 |
| 2 | 0 | 0.0025 | 0.8 | 0.0020 |
| 3 | 0 | 0.0025 | 0.8 | 0.0020 |
| 4 | 0 | 0.0025 | 0.8 | 0.0020 |
| 5 | 0 | 0.0025 | 0.8 | 0.0020 |
| 6 | 0 | 0.0025 | 0.8 | 0.0020 |
| 7 | 0 | 0.0025 | 0.8 | 0.0020 |
| 8 | 0 | 0.0025 | 0.8 | 0.0020 |
| 9 | 0 | 0.0025 | 0.8 | 0.0020 |
| 10 | 0 | 0.0025 | 0.8 | 0.0020 |
| 11 | 0 | 0.0025 | 0.8 | 0.0020 |
| 12 | 0 | 0.0025 | 0.8 | 0.0020 |
| 13 | 0 | 0.0025 | 0.8 | 0.0020 |
| 14 | 0 | 0.0025 | 0.8 | 0.0020 |
| 15 | 0 | 0.0025 | 0.8 | 0.0020 |
| 16 | 0 | 0.0025 | 0.8 | 0.0020 |
| 17 | 0 | 0.0025 | 0.8 | 0.0020 |
| 18 | 0 | 0.0025 | 0.8 | 0.0020 |
| 19 | 0 | 0.0025 | 0.8 | 0.0020 |
| 20 | 6 | 0.0025 | 0.8 | 0.0020 |
| 21 | 8 | 0.0025 | 0.8 | 0.0020 |
| 22 | 10 | 0.0025 | 0.8 | 0.0020 |
| 23 | 10 | 0.0025 | 0.8 | 0.0020 |
| 24 | 14 | 0.0025 | 0.8 | 0.0020 |
| Total | 52 | 0.0600 | 0.8 | 0.0480 |

# Bayesian Inference for Gamma-Poisson Model

$$\underbrace{P\left(\lambda_{post}/X\right)}_{Posterior} = \mathcal{G}(\underbrace{X+\alpha_{prior}}_{\alpha_{post}}, \overbrace{E+\beta_{prior}}^{\beta_{post}}) = \frac{\underbrace{\frac{(\lambda\cdot E)^X}{X!}e^{-\lambda\cdot E}}_{Likelihood}\cdot\underbrace{\frac{\beta_{prior}^{\alpha_{prior}}\cdot\lambda^{\alpha_{prior}-1}\cdot e^{-\lambda\cdot\beta_{prior}}}{\Gamma\left(\alpha_{prior}\right)}}_{Prior}}{\underbrace{\int_0^\infty \underbrace{\frac{(\lambda\cdot E)^X}{X!}e^{-\lambda\cdot E}}_{Likelihood}\cdot\underbrace{\frac{\beta_{prior}^{\alpha_{prior}}\cdot\lambda^{\alpha_{prior}-1}\cdot e^{-\lambda\cdot\beta_{prior}}}{\Gamma\left(\alpha_{prior}\right)}}_{Prior}d\lambda}_{Evidence}}$$

$$P_J(\lambda) = \mathcal{G}(\lambda; 0.5,0),\ \alpha = 0.5,\ \beta = 0$$

$$E\left(\lambda_{post}\right) = \frac{\alpha_{post}}{\beta_{post}} = \frac{\alpha_{prior}+X}{\beta_{prior}+E} = \frac{0.5+X}{E}$$

$$Var\left(\lambda_{post}\right) = \frac{\alpha_{post}}{\beta_{post}{}^2} = \frac{E\left(\lambda_{post}\right)}{\beta_{post}} = \frac{E\left(\lambda_{post}\right)}{E}$$

# Posterior Predictive Distribution for Gamma-Poisson Model

$$\underbrace{\mathrm{NB}\left(\tilde{x}; X, \alpha_{post}, \underbrace{\frac{\beta_{post}}{\beta_{post}+\tilde{A}}}_{p}\right)}_{\text{Predictive}} = \int_0^\infty \underbrace{\frac{(\lambda\cdot\tilde{A})^{\tilde{x}}}{\tilde{A}!} e^{-\lambda\cdot\tilde{A}}}_{\text{Likelihood}} \cdot \underbrace{\frac{\beta_{post}{}^{\alpha_{post}}\cdot\lambda^{\alpha_{post}-1}\cdot e^{-\lambda\cdot\beta_{post}}}{\Gamma(\alpha_{post})}}_{\text{Posterior}}$$

$$E(\tilde{x}) = \frac{\alpha_{post}}{\beta_{post}}\cdot\tilde{A} = \frac{0.5+X}{E}\cdot\tilde{A} = (0.5+X)\cdot\frac{\tilde{A}}{E} = E(\lambda_{post})\cdot\tilde{A}$$

$$Var(\tilde{x}) = E(\tilde{x})\cdot(1+\frac{\tilde{A}}{E})$$

# Treatment of zeros by different priors

| Prior | α,β | E(λ\|x) | E(λ\|X=0) |
|---|---|---|---|
| Jeffreys | Gamma(0.5,0) | $\frac{x+\alpha}{e+\beta}=\frac{x}{e}+\frac{0.5}{e}$ | $\frac{0.5}{e}$ |
| Uniform | Gamma(1,0) | $\frac{x+\alpha}{e+\beta}=\frac{x}{e}+\frac{1}{e}$ | $\frac{1}{e}$ |
| Max Entropy | Gamma(1,1/μ) | $\frac{\mu(x+1)}{e\cdot\mu+1}$ | $\frac{\mu}{e\cdot\mu+1}$ |
| Constrained noninformative (CNI) | Gamma(0.5, 1/(2·μ)) | $\frac{2\cdot\mu(x+0.5)}{2\cdot e\cdot\mu+1}$ | $\frac{\mu}{2\cdot e\cdot\mu+1}$ |
| Gamma prior | Gamma(α, β) | $\frac{x+\alpha}{e+\beta}$ | $\frac{\alpha}{e+\beta}$ |

- Previous missions have treated zero CFU results by adding 1 CFU at the Assay or Grouping level
  - Doesn't take into account sampled area (exposure)
- Bayesian treatment of a zero provides methods to estimate the bioburden density without drastic manipulation of the data

# Parameters of Gamma Distribution for Different Non-Informative Priors

| Prior distribution | α- shape | β - rate | Mean | Variance |
|---|---|---|---|---|
| Jeffreys | 0.5 | 0 | undefined | undefined |
| CNI | 0.5 | $1/(2 \cdot \mu)$ | μ | $2 \cdot \mu^2$ |
| MaxEnt | 1 | $1/\mu$ | μ | $\mu^2$ |
| Uniform | 1 | 0 | undefined | undefined |

# Summary of Bioburden Data for Eight InSight Components.

| Component | CFU Count | Area Sampled, $m^2$ | Exposure: Area Sampled*Pour Fraction, $m^2$ | Total Surface of the Component, $m^2$ | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|
| 9 | 0 | 0.6031 | 0.2167 | 0.7580 | 79.5650 |
| 73 | 0 | 2.4200 | 0.6160 | 2.7400 | 88.3212 |
| 300 | 1 | 2.6600 | 0.6705 | 5.0000 | 53.2000 |
| 169 | 1 | 0.2400 | 0.1920 | 0.5850 | 41.0260 |
| 283 | 5 | 4.5710 | 1.1427 | 12.0000 | 38.0920 |
| 243 | 5 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |
| 38 | 12 | 3.1050 | 0.8065 | 10.0000 | 31.0500 |
| 261 | 52 | 0.0600 | 0.0480 | 0.3120 | 19.2310 |

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# Summary of Posterior and Predictive Inference for Components 9,73,300

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 2.3064 | 0.0090 | 8.8600 | 1.7482 | 0 | 7 |
| CNI | 2.2889 | 0.0090 | 8.7928 | 1.7350 | 0 | 7 |
| MaxEnt | 4.5432 | 0.2330 | 13.6102 | 3.4437 | 0 | 11 |
| Uniform | 4.6128 | 0.2366 | 13.8189 | 3.4965 | 0 | 11 |

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 0.8116 | 0.0031 | 3.1180 | 2.2239 | 0 | 9 |
| CNI | 0.8094 | 0.0031 | 3.1096 | 2.2180 | 0 | 9 |
| MaxEnt | 1.6146 | 0.0828 | 4.8370 | 4.4241 | 0 | 14 |
| Uniform | 1.6233 | 0.0832 | 4.8631 | 4.4479 | 0 | 14 |

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 2.2371 | 0.2623 | 5.8274 | 11.1855 | 1 | 30 |
| CNI | 2.2315 | 0.2617 | 5.8130 | 11.1579 | 1 | 30 |
| MaxEnt | 2.9680 | 0.5273 | 7.0401 | 14.8404 | 2 | 37 |
| Uniform | 2.98280 | 0.5299 | 7.0750 | 14.9140 | 2 | 37 |

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# Summary of Posterior and Predictive Inference for Components 169,283,243

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 7.8120 | 0.9162 | 20.3497 | 4.5700 | 0 | 13 |
| CNI | 7.7452 | 0.9083 | 20.1757 | 4.5309 | 0 | 13 |
| MaxEnt | 10.2389 | 1.8192 | 24.2859 | 5.9897 | 0 | 15 |
| Uniform | 10.4161 | 1.8507 | 24.7063 | 6.0934 | 0 | 16 |

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 4.8129 | 2.0016 | 8.6086 | 57.7549 | 22 | 105 |
| CNI | 4.8059 | 1.9987 | 8.5961 | 57.6713 | 22 | 105 |
| MaxEnt | 5.2352 | 2.2799 | 9.1730 | 62.8226 | 26 | 112 |
| Uniform | 5.2504 | 2.2865 | 9.1996 | 63.0053 | 26 | 113 |

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m² | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | Predictive Mean, CFU | 5th Percentile of Predictive Distribution | 95th Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 48.2413 | 20.0632 | 86.2868 | 14.3759 | 5 | 28 |
| CNI | 47.5504 | 19.7758 | 85.0510 | 14.1700 | 4 | 27 |
| MaxEnt | 51.1363 | 22.2700 | 89.5997 | 15.2386 | 5 | 29 |
| Uniform | 52.6269 | 22.9191 | 92.2115 | 15.6828 | 5 | 30 |

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# Summary of Posterior and Predictive Inference for Components 38,261

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m$^2$ | 5$^{th}$ Percentile of Posterior Distribution | 95$^{th}$ Percentile of Posterior Distribution | Predictive Mean, CFU | 5$^{th}$ Percentile of Predictive Distribution | 95$^{th}$ Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 15.4988 | 9.0584 | 23.3428 | 154.9887 | 88 | 237 |
| CNI | 15.4671 | 9.0398 | 23.2949 | 154.6710 | 88 | 236 |
| MaxEnt | 16.0526 | 9.4952 | 24.0081 | 160.5268 | 92 | 243 |
| Uniform | 16.1188 | 9.5343 | 24.1070 | 161.1883 | 93 | 244 |

| Prior Distribution | Posterior Mean Bioburden Density – λ, CFU/m$^2$ | 5$^{th}$ Percentile of Posterior Distribution | 95$^{th}$ Percentile of Posterior Distribution | Predictive Mean, CFU | 5$^{th}$ Percentile of Predictive Distribution | 95$^{th}$ Percentile of Predictive Distribution |
|---|---|---|---|---|---|---|
| Jeffreys | 1093.5221 | 857.6728 | 1353.0301 | 341.1789 | 262 | 428 |
| CNI | 1057.0469 | 829.0645 | 1307.8988 | 329.7986 | 253 | 414 |
| MaxEnt | 1032.4675 | 810.7817 | 1276.2804 | 322.1298 | 248 | 404 |
| Uniform | 1103.9366 | 866.9054 | 1364.6267 | 344.4282 | 265 | 432 |

# Comparison of Bayesian Posterior Inference Using CNI Prior with NASA Weighted Average and 3-σ Approaches for the Eight Components.

| | Proposed Bayesian Approach | | | MSL-based 3 sigma (NASA Legacy) | InSight-based weighted average technique (NASA Current) |
|---|---|---|---|---|---|
| Component | Posterior Mean Bioburden Density – λ, CFU/$m^2$ | 5th Percentile of Posterior Distribution | 95th Percentile of Posterior Distribution | 3 sigma Bioburden Density – λ, CFU/$m^2$ | Weighted Average Bioburden Density – λ, CFU/$m^2$ |
| **9** | 2.2889 | 0.0090 | 8.7928 | 13.84 | 27.99 |
| **73** | 0.8095 | 0.0032 | 3.1097 | 4.87 | 17.36 |
| **300** | 2.2315 | 0.2617 | 5.8130 | 5.96 | 9.54 |
| **169** | 7.7452 | 0.9083 | 20.1757 | 20.83 | 33.70 |
| **283** | 4.8059 | 1.9987 | 8.5961 | 5.17 | 11.11 |
| **243** | 47.5504 | 19.7758 | 85.0510 | 130.14 | 186.70 |
| **38** | 15.4671 | 9.0398 | 23.2949 | 52.06 | 9.66 |
| **261** | 1057.0469 | 829.0645 | 1307.8988 | 2349.53 | 658.47 |

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# Bayesian Parameter Estimation

## Bayesian inference

$$\pi(\lambda/x, \alpha) = \frac{L(x/\lambda)\cdot\pi(\lambda/\alpha)}{\int L(x/\lambda)\cdot\pi(\lambda/\alpha)d\lambda}$$

## Prior predictive distribution

$$\pi(x/\alpha) = \int_0^\infty L(x/\lambda)\cdot\pi(\lambda/\alpha)d\lambda$$

## Posterior predictive distribution

$$\pi(x/\alpha) = \int_0^\infty L(x/\lambda)\cdot\pi(\lambda/x, \alpha)d\lambda$$

## Empirical Bayes (Method of Moments-MOM)

$$\pi(\lambda/x, \hat{\alpha}) = \frac{L(x/\lambda)\cdot\pi(\lambda/\hat{\alpha})}{\int L(x/\lambda)\cdot\pi(\lambda/\hat{\alpha})d\lambda}$$

## Hierarchical Bayes

$$\pi(\lambda/x, \alpha) = \frac{L(x/\lambda)\cdot\pi(\lambda/\alpha)\cdot h(\alpha)}{\int L(x/\lambda)\cdot\pi(\lambda/\alpha)\cdot h(\alpha)d\lambda d\alpha}$$

# Summary of posterior and predictive inference for components 9, 73, 300

**9**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 2.2889 | 0.0090 | 8.7928 | 1.7350 | 0 | 7 |
| MOM | 0.7603 | 4.1117e-08 | 4.0993 | 0.5763 | 0 | 3 |

**73**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 0.8094 | 0.0031 | 3.1096 | 2.2180 | 0 | 9 |
| MOM | 0.2684 | 1.4519e-08 | 1.4475 | 0.7356 | 0 | 4 |

**300**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 2.2315 | 0.2617 | 5.8130 | 11.1579 | 1 | 30 |
| MOM | 1.7355 | 0.1267 | 4.9272 | 8.6778 | 0 | 26 |

# Summary of posterior and predictive inference for components 169, 283, 243

**169**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 7.7452 | 0.9083 | 20.1757 | 4.5309 | 0 | 13 |
| MOM | 6.0352 | 0.4408 | 17.1337 | 3.5305 | 0 | 11 |

**283**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 4.8059 | 1.9987 | 8.5961 | 57.6713 | 22 | 105 |
| MOM | 4.5158 | 1.8133 | 8.2011 | 54.1903 | 20 | 100 |

**243**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m² | 5th percentile of posterior distribution | 95th percentile of posterior distribution | Predictive mean, CFU | 5th percentile of predictive distribution | 95th percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 47.5504 | 19.7758 | 85.0510 | 14.1700 | 4 | 27 |
| MOM | 44.8607 | 18.0138 | 81.4700 | 13.3685 | 4 | 26 |

# Summary of posterior and predictive inference for components 38, 261

**38**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m$^2$ | 5$^{th}$ percentile of posterior distribution | 95$^{th}$ percentile of posterior distribution | Predictive mean, CFU | 5$^{th}$ percentile of predictive distribution | 95$^{th}$ percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 15.4671 | 9.0398 | 23.2949 | 154.6710 | 88 | 236 |
| MOM | 15.0630 | 8.7294 | 22.7980 | 150.6308 | 85 | 231 |

**261**

| Prior distribution | Posterior mean. Bioburden density – λ, CFU/m$^2$ | 5$^{th}$ percentile of posterior distribution | 95$^{th}$ percentile of posterior distribution | Predictive mean, CFU | 5$^{th}$ percentile of predictive distribution | 95$^{th}$ percentile of predictive distribution |
|---|---|---|---|---|---|---|
| CNI | 1057.0469 | 829.0645 | 1307.8988 | 329.7986 | 253 | 414 |
| MOM | 1061.3672 | 831.7609 | 1314.0833 | 331.1465 | 254 | 416 |

# Bioburden Density Comparison

| | Proposed Bayesian Approach | | MSL-based 3 sigma (NASA Legacy) | InSight-based weighted average technique (NASA Current) |
|---|---|---|---|---|
| **Component** | CNI, Posterior Mean Bioburden Density – λ, CFU/$m^2$ | MOM, Posterior Mean Bioburden Density – λ, CFU/m2 | 3 sigma Bioburden Density – λ, CFU/$m^2$ | Weighted Average Bioburden Density – λ, CFU/$m^2$ |
| **9** | 2.2889 | 0.7603 | 13.84 | 27.99 |
| **73** | 0.8094 | 0.2684 | 4.87 | 17.36 |
| **300** | 2.2315 | 1.7355 | 5.96 | 9.54 |
| **169** | 7.7452 | 6.0352 | 20.83 | 33.70 |
| **283** | 4.8059 | 4.5158 | 5.17 | 11.11 |
| **243** | 47.5504 | 44.8607 | 130.14 | 186.70 |
| **38** | 15.4671 | 15.0630 | 52.06 | 9.66 |
| **261** | 1057.0469 | 1061.3672 | 2349.53 | 658.47 |

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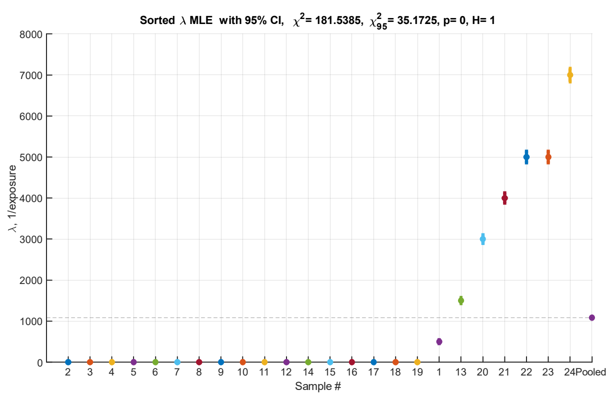
# Summary of Bioburden Data for the Eight InSight Components

| Component | CFU Count | Number of Samples | Area Sampled, $m^2$ | Total Exposure: Area Sampled*Pour Fraction, $m^2$ | Total Surface of the Component, $m^2$ | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|---|
| 9 | 0 | 49 | 0.6031 | 0.2167 | 0.7580 | 79.5650 |
| 38 | 12 | 27 | 3.1050 | 0.8065 | 10.0000 | 31.0500 |
| 67 | 0 | 27 | 2.4200 | 0.6160 | 2.7400 | 88.3212 |
| 169 | 1 | 17 | 0.2400 | 0.1920 | 0.5850 | 41.0260 |
| 243 | 5 | 34 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |
| **261** | **52** | **24** | **0.0600** | **0.0480** | **0.3120** | **19.2310** |
| 283 | 5 | 8 | 4.5710 | 1.1427 | 12.0000 | 38.0920 |
| 300 | 1 | 9 | 2.6600 | 0.6705 | 5.0000 | 53.2000 |




$$P(X = x|\lambda) = \frac{(\lambda \cdot E)^x}{x!} \cdot e^{-\lambda \cdot E}, \lambda \geq 0, x = 0,1,\ldots$$

$$\hat{\lambda}_i^{MLE} = \frac{x_i}{E_i}, i = 1, \ldots N$$

$$\hat{\lambda}_{pooled}^{MLE} = \frac{\sum_{i=1}^{N} x_i}{\sum_{i=1}^{N} E_i}$$

| Component 261 Sample # | CFUs observed | Area sampled, $m^2$ | Pour fraction | Exposure, $m^2$ |
|---|---|---|---|---|
| 1 | 1 | 0.0025 | 0.8 | 0.0020 |
| 2 | 0 | 0.0025 | 0.8 | 0.0020 |
| 3 | 0 | 0.0025 | 0.8 | 0.0020 |
| 4 | 0 | 0.0025 | 0.8 | 0.0020 |
| 5 | 0 | 0.0025 | 0.8 | 0.0020 |
| 6 | 0 | 0.0025 | 0.8 | 0.0020 |
| 7 | 0 | 0.0025 | 0.8 | 0.0020 |
| 8 | 0 | 0.0025 | 0.8 | 0.0020 |
| 9 | 0 | 0.0025 | 0.8 | 0.0020 |
| 10 | 0 | 0.0025 | 0.8 | 0.0020 |
| 11 | 0 | 0.0025 | 0.8 | 0.0020 |
| 12 | 0 | 0.0025 | 0.8 | 0.0020 |
| 13 | 3 | 0.0025 | 0.8 | 0.0020 |
| 14 | 0 | 0.0025 | 0.8 | 0.0020 |
| 15 | 0 | 0.0025 | 0.8 | 0.0020 |
| 16 | 0 | 0.0025 | 0.8 | 0.0020 |
| 17 | 0 | 0.0025 | 0.8 | 0.0020 |
| 18 | 0 | 0.0025 | 0.8 | 0.0020 |
| 19 | 0 | 0.0025 | 0.8 | 0.0020 |
| 20 | 6 | 0.0025 | 0.8 | 0.0020 |
| 21 | 8 | 0.0025 | 0.8 | 0.0020 |
| 22 | 10 | 0.0025 | 0.8 | 0.0020 |
| 23 | 10 | 0.0025 | 0.8 | 0.0020 |
| 24 | 14 | 0.0025 | 0.8 | 0.0020 |
| Total | 52 | 0.0600 | 0.8 | 0.0480 |

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# Data Generating Model and Parameter Estimators

$$X_i = x|\lambda_{true}^i \sim Poisson(\lambda_{true}^i \cdot E_i)$$

$$\lambda_{true}^i|\alpha, \beta \sim Gamma(\alpha, \beta), i = 1, \dots N$$

$\widehat{\lambda_i}(x_i) = \frac{x_i}{E_i}$ - Maximum Likelihood Estimator (MLE)

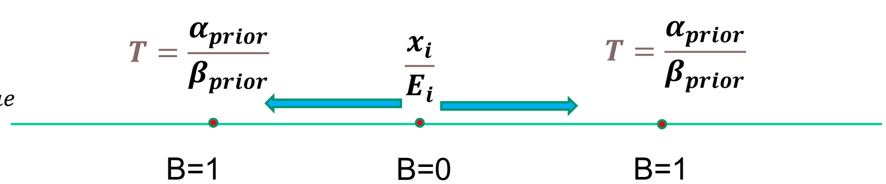
$\widehat{\lambda_i}(x_i) = \frac{x_i+\alpha}{E_i+\beta}$ - Conjugate prior Bayes Estimator

$\widehat{\lambda_i} = d$ - Deterministic Estimator

$X_i$ – random variable describing the number of CFUs on i-th sampled component
$x_i$ – observed number of CFUs in a sample from i-th sampled component
$E_i$ – exposure for a sample, determined by multiplying the sampled area by pour fraction
$\lambda_{true}^i$– true bioburden density for a sample
$Gamma(\lambda / \alpha,\beta)$ – Gamma prior distribution of bioburden density $\lambda_{true}^i$
α,β – parameters of the Gamma prior distribution
$Poisson(\lambda_{true}^i \cdot E_i)$– Poisson likelihood of having x CFU counts at exposure $E_i$ given $\lambda_{true}^i$
N-number of components

- Bayesian and Deterministic estimators are shrinkage estimators with respect to MLE
- Shrinkage estimators pulls MLE towards a prespecified target value
- Shrinkage reduces the variance of the estimate at the expense of introducing bias
- Variance reduction can outweigh increase in bias thus improving mean squared error of the estimator

$$\widehat{\lambda_i} = \frac{x_i}{E_i} - B \cdot \left(\frac{x_i}{E_i} - T\right) \quad B = \frac{\beta_{prior}}{E_i + \beta_{prior}} \leq 1$$

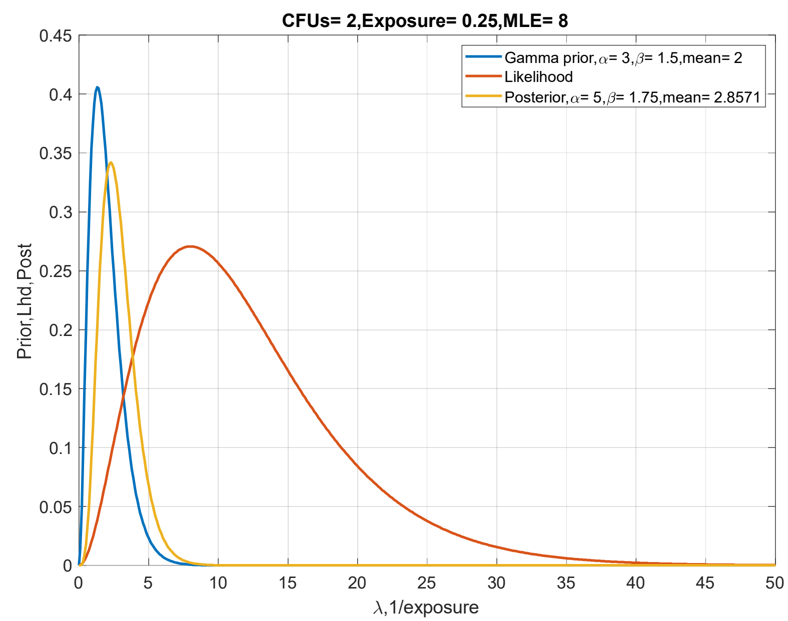


# Gamma-Poisson Model

$$P(\lambda/x) = \frac{\underbrace{\frac{(\lambda\cdot e)^x}{x!}e^{-\lambda\cdot e}}_{Likelihood}.\underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}}.\lambda^{\alpha_{prior}-1}.e^{-\lambda\cdot\beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior}}{\int_0^\infty \underbrace{\frac{(\lambda\cdot e)^x}{x!}e^{-\lambda\cdot e}}_{Likelihood}.\underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}}.\lambda^{\alpha_{prior}-1}.e^{-\lambda\cdot\beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior}d\lambda} = Gamma(\underbrace{x+\alpha_{prior}}_{\alpha_{post}}, \overbrace{e+\beta_{prior}}^{\beta_{post}})$$

$$E_{prior}(\lambda/\alpha_{prior},\beta_{prior}) = \frac{\alpha_{prior}}{\beta_{prior}}$$

$$E_{post}(\lambda/x,\alpha_{prior},\beta_{prior}) = \frac{\underbrace{x+\alpha_{prior}}_{\alpha_{post}}}{\overbrace{e+\beta_{prior}}^{\beta_{post}}}$$



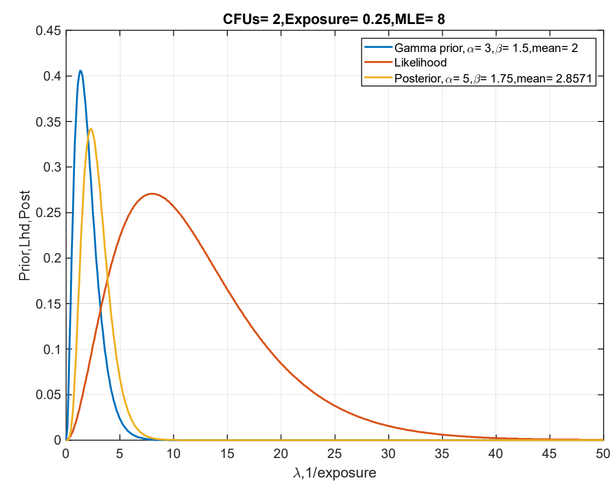
# Different Types of Prior

$$E_{post}\left(\lambda/x,\alpha_{prior},\beta_{prior}\right)=\frac{\underbrace{x+\alpha_{prior}}_{\alpha_{post}}}{\overbrace{\mathrm{e}+\beta_{prior}}^{\beta_{post}}}$$

$$E(\lambda|x)=\frac{x+\alpha_{prior}}{\mathrm{e}+\beta_{prior}}=\left[\frac{e}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e}\right)+\left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right)=[1-B]\cdot\left(\frac{x}{e}\right)+[B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$=\left(\frac{x}{e}\right)-[B]\cdot\left(\frac{x}{e}-\frac{\alpha_{prior}}{\beta_{prior}}\right)=\left(\frac{x}{e}\right)-\left[\frac{\beta}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e}-\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B=\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\leq 1$$



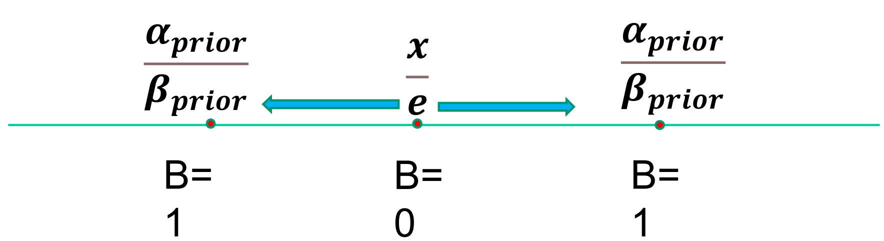
# Shrinkage as Partial Pooling

$$E(\lambda|x) = \frac{x+\alpha_{prior}}{\mathrm{e}+\beta_{prior}} = \left[\frac{e}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e}\right) + \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$= \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\lambda)}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}} \leq 1 \qquad \lim_{\beta_{prior}\to 0}\frac{\beta_{prior}}{e+\beta_{prior}} = 0 \qquad \lim_{\beta_{prior}\to\infty}\frac{\beta_{prior}}{e+\beta_{prior}} = 1 \qquad E(\lambda) = \frac{\alpha}{\beta}, Var(\lambda) = \frac{\alpha}{\beta^2}$$

$$\lim_{e\to 0}\frac{\beta_{prior}}{e+\beta_{prior}} = 1 \qquad \lim_{e\to\infty}\frac{\beta_{prior}}{e+\beta_{prior}} = 0$$



# Data Poolability, Shrinkage Estimators, and Risk

$$\underbrace{P(\lambda_{post}/x)}_{Posterior} = \mathcal{G}\left(\underbrace{x+\alpha_{prior}}_{\alpha_{post}}, \overbrace{E+\beta_{prior}}^{\beta_{post}}\right) = \frac{\underbrace{\frac{(\lambda\cdot E)^x}{x!}e^{-\lambda\cdot E}}_{Likelihood}\cdot\underbrace{\frac{\beta_{prior}^{\alpha_{prior}}\cdot\lambda^{\alpha_{prior}-1}\cdot e^{-\lambda\cdot\beta_{prior}}}{\Gamma\left(\alpha_{prior}\right)}}_{Prior}}{\underbrace{\int_0^\infty \underbrace{\frac{(\lambda\cdot E)^x}{x!}e^{-\lambda\cdot E}}_{Likelihood}\cdot\underbrace{\frac{\beta_{prior}^{\alpha_{prior}}\cdot\lambda^{\alpha_{prior}-1}\cdot e^{-\lambda\cdot\beta_{prior}}}{\Gamma\left(\alpha_{prior}\right)}}_{Prior}d\lambda}_{Evidence}}$$

$$E(\lambda|x) = \frac{x+\alpha_{prior}}{E+\beta_{prior}} = \left[\frac{e}{E+\beta_{prior}}\right]\cdot\left(\frac{x}{E}\right) + \left[\frac{\beta_{prior}}{E+\beta_{prior}}\right]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = [1-B]\cdot\left(\frac{x}{E}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = \left(\frac{\boldsymbol{x}}{\boldsymbol{E}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{E}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{E_{prior}(\lambda)}\right)$$

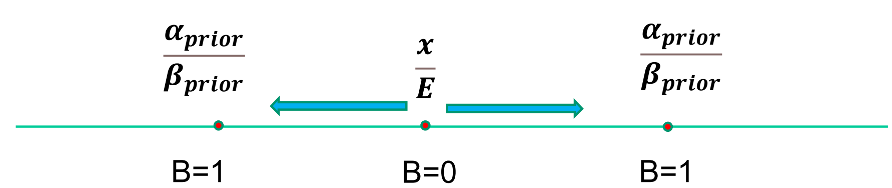
$$= \left(\frac{x}{E}\right) - \left[\frac{\beta_{prior}}{E+\beta_{prior}}\right]\cdot\left(\frac{x}{E} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{E+\beta_{prior}} \le 1 \qquad \lim_{\beta_{prior}\to 0}\frac{\beta_{prior}}{E+\beta_{prior}} = 0 \qquad \lim_{\beta_{prior}\to \infty}\frac{\beta_{prior}}{E+\beta_{prior}} = 1 \qquad \lim_{E\to 0}\frac{\beta_{prior}}{E+\beta_{prior}} = 1 \qquad \lim_{E\to \infty}\frac{\beta_{prior}}{E+\beta_{prior}} = 0$$

$$E(\lambda) = \frac{\alpha}{\beta}, Var(\lambda) = \frac{\alpha}{\beta^2} \qquad L\left(\lambda_{true}, \hat{\lambda}(x)\right) = \left(\lambda_{true} - \hat{\lambda}(x)\right)^2 \qquad R\left(\lambda_{true}, \hat{\lambda}(x)\right) = \sum_x \left(\lambda_{true} - \hat{\lambda}(x)\right)^2 \cdot p(x;\lambda_{true})$$

$$\hat{\lambda}_i = \frac{x_i}{E_i} - B\cdot\left(\frac{x_i}{E_i} - T\right), i = 1, \ldots N \qquad \hat{\lambda}_i = \frac{x_i}{E_i} - B\cdot\left(\frac{x_i}{E_i}\right), i = 1, \ldots N$$

- Pooling is the process of grouping the data according to the values of bioburden density λ.
- Data poolability can be statistically tested.
- How can the data be grouped to minimize risk?
- Shrinkage estimators perform partial pooling of the data and reduce risk.
- Roughly only 10% of the spacecraft is sampled.
- A constant estimator is an extreme example of a shrinkage estimator.
- Constant estimators are used for both specified and implied components.
- Bayesian estimators are shrinkage estimators.
- Risk is a measure of how far our estimate from the true and unknown values of bioburden density.
- In the current work, the mean squared error (MSE) is assumed as a risk function.



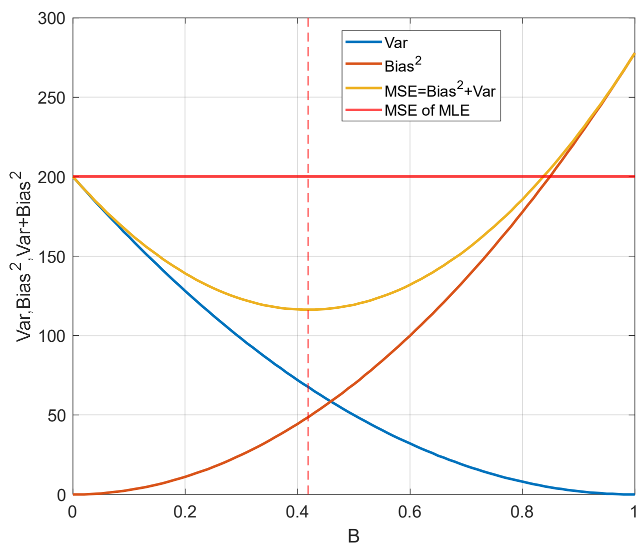
# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein), Borrowing Information

$$E(\hat{\lambda}_{JS}|x) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}(\lambda)}}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$MSE_{JS} = \frac{\lambda_{true}}{e}\cdot(1-B)^2 + \left(B\cdot\left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$$

$$\frac{\alpha_{prior}}{\beta_{prior}} = 33.3\ \mathrm{CFUs}/m^2$$

$$\lambda_{true} = 50\ \mathrm{CFUs}/m^2$$

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# Estimators' Loss Functions and Risks

$$L\left(\hat{\lambda}_i(x), \lambda_{true}^i\right) = \left(\hat{\lambda}_i(x) - \lambda_{true}^i\right)^2 - Loss\ function\ for\ a\ data - driven\ estimators, \text{(MLE and Bayes)}$$

$$L\left(\hat{\lambda}_i, \lambda_{true}^i\right) = \left(\hat{\lambda}_i - \lambda_{true}^i\right)^2 - Loss\ function\ for\ a\ deterministic\ estimator$$

$$R_{Frequentist}\left(\lambda_{true}^i, \hat{\lambda}_i(x)\right) = \sum_x \left(\lambda_{true}^i - \hat{\lambda}_i(x)\right)^2 \cdot p\left(x; \lambda_{true}^i\right) = \sum_{x=0}^{\infty} \left(\lambda_{true}^i - \hat{\lambda}_i(x)\right)^2 \cdot \frac{\left(\lambda_{true}^i \cdot E_i\right)^x}{x!} \cdot e^{-\lambda_{true}^i \cdot E_i}$$

$$\rho_{Posterior\ expected\ loss}\left(\alpha, \beta, x_i, \hat{\lambda}_i(x)\right) = \int_0^{\infty} \left(\lambda_{true}^i - \hat{\lambda}_i(x_i)\right)^2 \cdot Gamma(\lambda_{true}^i | x_i, \alpha, \beta) d\lambda_{true}^i$$

$$r_{Integrated}\left(\alpha, \beta, \hat{\lambda}_i\right) = \int_0^{\infty} R\left(\lambda_{true}^i, \hat{\lambda}_i(x)\right) \cdot Gamma(\lambda_{true}^i | x_i, \alpha, \beta) d\lambda_{true}^i = \sum_{x=0}^{\infty} \rho\left(\alpha, \beta, x_i, \hat{\lambda}_i(x)\right) \cdot NB\left(x | \alpha, \frac{\beta}{\beta + E_i}\right)$$

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# Risks for Three Different Estimators

| Estimator | R-Frequentist Risk | ρ-Posterior Expected Loss | r- Integrated Risk |
|---|---|---|---|
| $d$ (deterministic) | $(d-\lambda_{true})^2$ | $\frac{\alpha}{\beta^2}+\left(d-\frac{\alpha}{\beta}\right)^2$ | $\frac{\alpha}{\beta^2}+\left(d-\frac{\alpha}{\beta}\right)^2$ |
| $\frac{x}{E}$ (MLE) | $\frac{\lambda_{true}}{E}$ | $\frac{x+\alpha}{(E+\beta)^2}+\left(\frac{x}{E}-\frac{\alpha}{\beta}\right)^2$ | $\frac{\alpha}{E\cdot\beta}$ |
| $\frac{x+\alpha}{E+\beta}$ (Bayes) | $\frac{\lambda_{true}}{E}\cdot(1-B)^2+\left(B\cdot\left(\lambda_{true}-\frac{\alpha}{\beta}\right)\right)^2$ <br> $B=\frac{\beta}{\mathrm{E}+\beta}\leq 1$ | $\frac{x+\alpha}{(E+\beta)^2}$ | $\frac{\alpha}{\beta\cdot(E+\beta)}$ |

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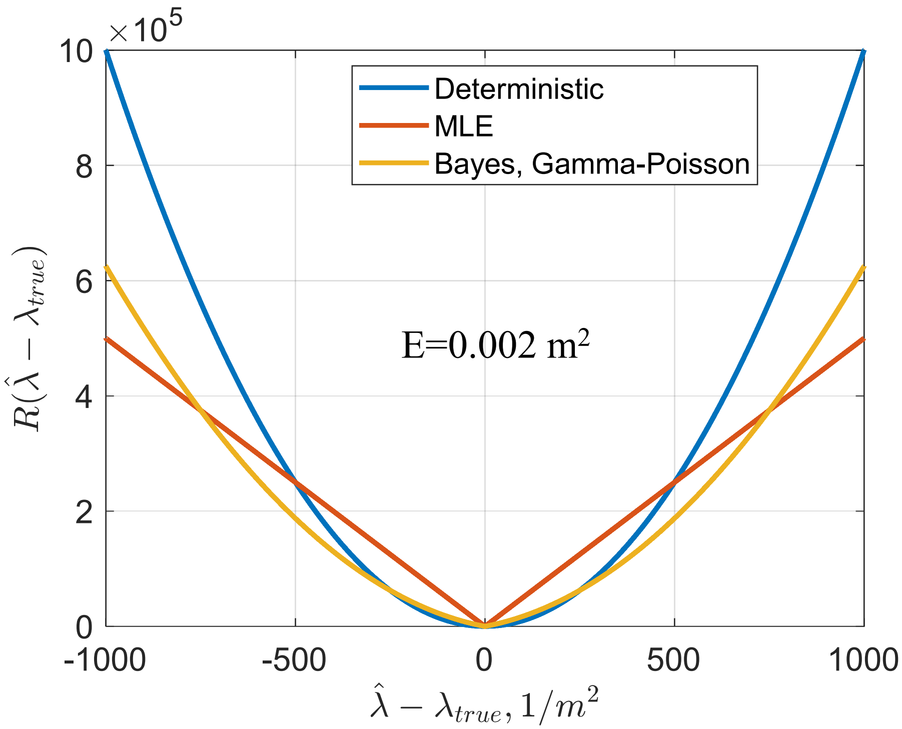
# Frequentist Risks of Three Estimators




| Estimator | R-Frequentist Risk |
|---|---|
| $d=1000$ (deterministic) | $(d - \lambda_{true})^2$ |
| $\frac{x}{E}$, (MLE) | $\frac{\lambda_{true}}{E}$ |
| $\frac{x+\alpha}{E+\beta}$ (Bayes) | $\frac{\lambda_{true}}{E} \cdot (1-B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha}{\beta}\right)\right)^2$ <br> $B = \frac{\beta}{E+\beta} \leq 1, \frac{\alpha}{\beta} = 1000 \frac{CFUs}{m^2}, B = 0.5$ |

Use case scenario: Given a specified value of 100 CFUs/m² with uncertainty 40 CFUs/m² for a component, and an opportunity to sample the component with one swab, it is better to use the specified value than to sample.

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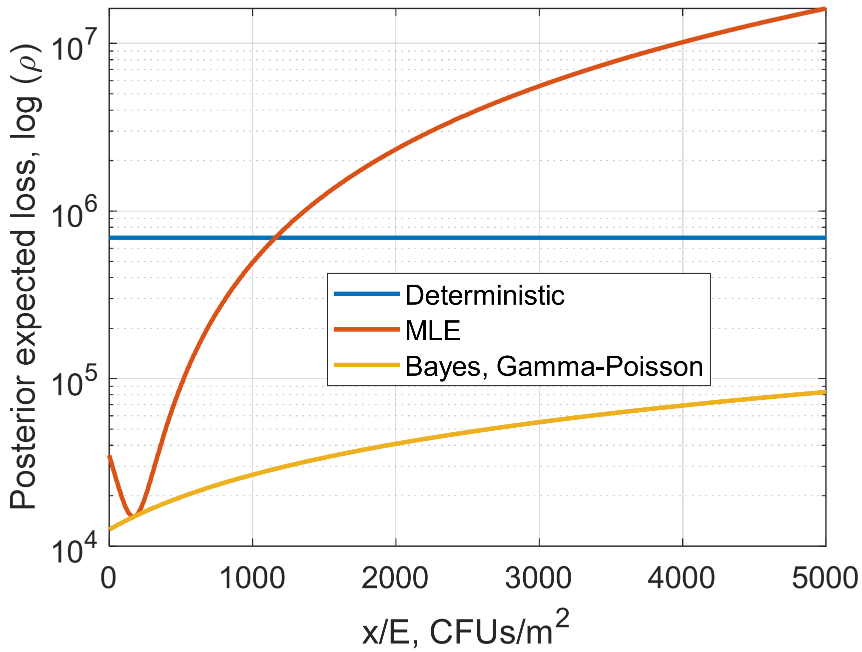
# Posterior Expected Loss of Three Estimators

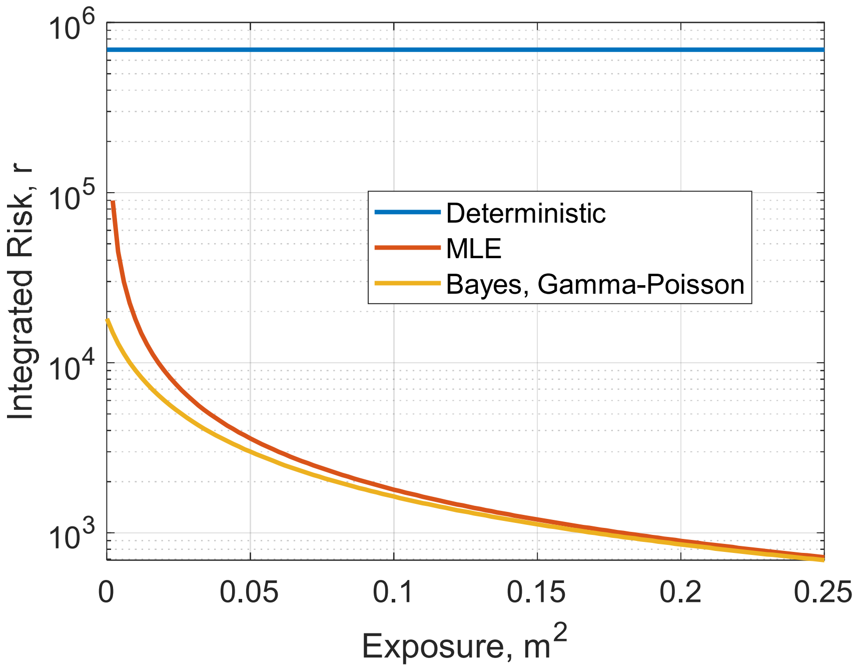



| Estimator | ρ-Posterior Expected Loss |
|---|---|
| *d=1000* (deterministic) | $\frac{\alpha}{\beta^2} + \left(d - \frac{\alpha}{\beta}\right)^2$ |
| $\frac{x}{E}$ (MLE) | $\frac{x+\alpha}{(E+\beta)^2} + \left(\frac{x}{E} - \frac{\alpha}{\beta}\right)^2$ |
| $\frac{x+\alpha}{E+\beta}$ (Bayes) | $\frac{x+\alpha}{(E+\beta)^2}$ |

Use case scenario: if x/E=1000 CFUs/m$^2$, then $\rho_{Bayes} \leq \rho_{MLE} \leq \rho_d$

$$\frac{\alpha}{\beta} = 179.58\ CFUs/m^2$$

# Integrated Risk of Three Estimators




| Estimator | r- Integrated Risk |
|---|---|
| *d=1000* (deterministic) | $\frac{\alpha}{\beta^2} + \left(d - \frac{\alpha}{\beta}\right)^2$ |
| $\frac{x}{E}$ (MLE) | $\frac{\alpha}{E \cdot \beta}$ |
| $\frac{x+\alpha}{E+\beta}$ (Bayes) | $\frac{\alpha}{\beta \cdot (E+\beta)}$ |

$$\frac{\alpha}{\beta} = 179.58\ CFUs/m^2$$

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# Integrated Risk and Sampling Size Determination

$$TR(E) = \frac{\alpha}{\beta \cdot (E + \beta)} + C_0 + C \cdot E$$

$$E_{opt} = max\left\{0, \sqrt{\frac{\alpha}{C \cdot \beta}} - \beta\right\}$$

| Implied Component # | Implied from Component # (implicant) | Implied Bioburden Density, $\hat{\lambda}$, CFU/m$^2$ | Implied Risk, CFUs/m$^2$ | Total Surface Area of the Implied Component, m$^2$ | Optimal Sampling Area, m$^2$ | Optimal Risk, CFUs/m$^2$ | Optimal Cost, $ |
|---|---|---|---|---|---|---|---|
| 2 | 10 | 12.05 | 17.03 | 0.256 | 0.162 | 7.68 | 126.80 |
| 106 | 108 | 13.51 | 19.11 | 0.533 | 0.178 | 7.91 | 138.78 |
| 133 | 131 | 5.10 | 4.16 | 0.013 | 0 | 4.16 | 0 |
| 36 | 38 | 15.50 | 4.38 | 2.0 | 0 | 4.38 | 0 |
| 71 | 70 | 2.47 | 2.02 | 7.0 | 0 | 2.02 | 0 |
| 29 | 32 | 104.16 | 65.88 | 0.166 | 0.166 | 23.41 | 129.46 |

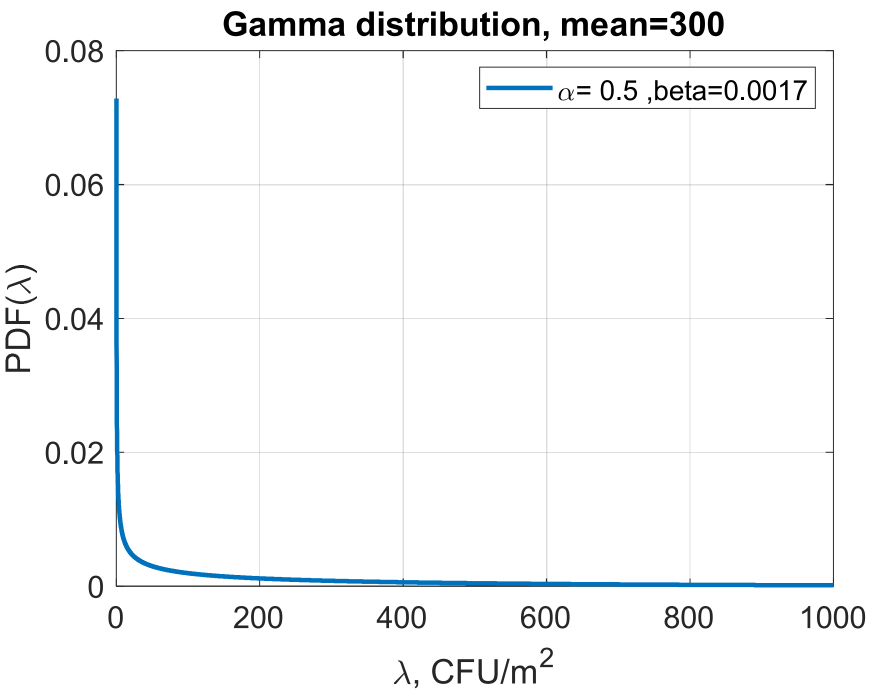
# Risks of Different Estimators

| Estimator | R- Bayes Risk |
|---|---|
| **0** | $\frac{\alpha}{\beta^2}+\left(\frac{\alpha}{\beta}\right)^2$ |
| **d** | $\frac{\alpha}{\beta^2}+\left(d-\frac{\alpha}{\beta}\right)^2$ |
| $\frac{x}{e}$ | $\frac{\alpha}{e\cdot\beta}$ |
| $\frac{x+\alpha}{e+\beta}$ | $\frac{\alpha}{\beta\cdot(e+\beta)}$ |

- Given an estimator, a loss function, and a prior we can calculate the risk
- Assume Gamma distribution prior with α as shape parameter and β as rate parameter: Gamma( α,β)
- Assume Poisson sampling model and symmetric squared error loss
- Calculate risks of deterministic estimators used for specified and implied components
- Specified bioburden is usually a number, sometimes (very rarely) it is a number with a range
- Implied component's bioburden has a distribution implied from another component
- Risks of bioburden estimation for sampled components can be controlled via exposure

$$P\left(X_i = x_i \middle| \lambda_{true}^i\right) = \frac{(\lambda_{true}^i)^{x_i}}{x_i!} e^{-\lambda_{true}^i \cdot e_i}, x = 0,1,2,\ldots, \lambda_{true} \in (0,\infty), e \in (0,\infty)$$

# Risk of Specified Estimator




For InSight data, the specification values range from 10 CFUs/$m^2$ to 10000 CFUs/$m^2$

Assume constrained noninformative prior (CNI) with mean value equal to the specified value, μ CFU/$m^2$

In this case prior is Gamma(α=0.5, $\beta = \frac{1}{2\cdot\mu}$)

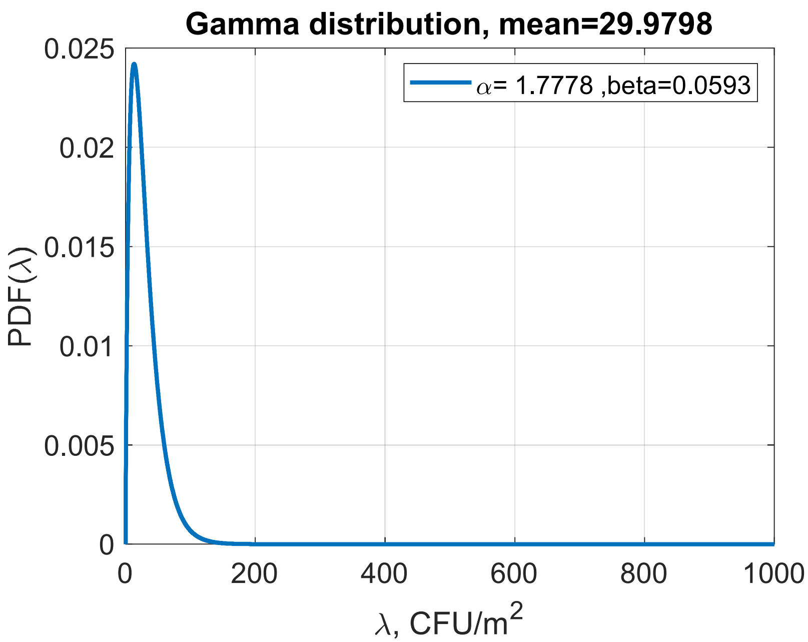
$$R(\alpha,\beta) = \frac{\alpha}{\beta^2} + \left(\mu - \frac{\alpha}{\beta}\right)^2 = \frac{\alpha}{\beta^2};\ \frac{0.5}{\left(\frac{1}{2\cdot\mu}\right)^2} = 2\cdot\mu^2$$

$$\sqrt{R(\alpha,\beta)} = \sqrt{2}\cdot\mu = \sqrt{2}\cdot 300\,\frac{CFU}{m^2} = 424.3\ \frac{CFU}{m^2}$$

$$\sqrt{R(\alpha,\beta)} = \sqrt{2}\cdot\mu = \sqrt{2}\cdot 10\,\frac{CFU}{m^2} = 14.2\ \frac{CFU}{m^2}$$

$$\sqrt{R(\alpha,\beta)} = \sqrt{2}\cdot\mu = \sqrt{2}\cdot 1000\,\frac{CFU}{m^2} = 1414.2\ \frac{CFU}{m^2}$$

# Risk of Specified Estimator with Given mean Value and Range




For InSight data, component 15 has specified value of mean , 30 CFU's/$m^2$ and range 10-100 CFU's/$m^2$

Using these values and approximation Var≈$(range/4)^2$

the prior is Gamma($\alpha$=1.7778, $\beta = 0.0593$)

$$R(\alpha,\beta) = \frac{\alpha}{\beta^2} + \left(\mu - \frac{\alpha}{\beta}\right)^2 = \frac{\alpha}{\beta^2};\ \frac{1.7778}{(0.0593)^2}$$

$$\sqrt{R(\alpha,\beta)} = 22.5\ \frac{CFU}{m^2}$$

$$\sqrt{R(\alpha,\beta)} = \sqrt{2}\cdot\mu = \sqrt{2}\cdot 30\frac{CFU}{m^2} = 42.4\ \frac{CFU}{m^2}$$

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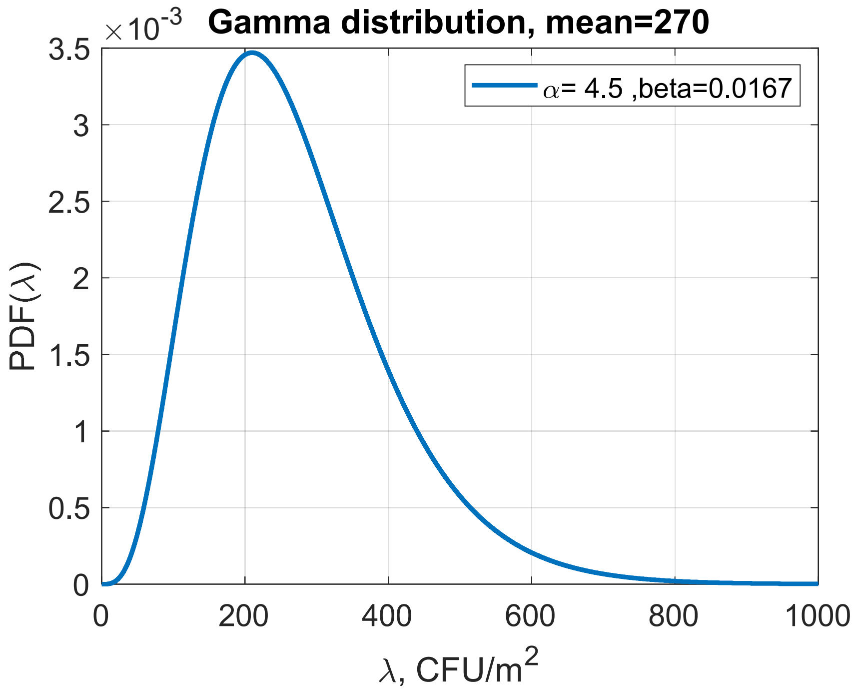
# Risk of Implied Estimators




$$R(\alpha,\beta) = \frac{\alpha}{\beta^2} + \left(\mu - \frac{\alpha}{\beta}\right)^2 = \frac{\alpha}{\beta^2};$$

$$\sqrt{R(\alpha,\beta)} = \sqrt{\frac{4.5}{(0.0167)^2}} = \sqrt{4.5} \cdot \frac{1}{0.0167} = 127.28\ \frac{CFU}{m^2}$$

# Sampling Design for an Implied Component

$$\sqrt{R(\alpha = 4.5, \beta = 0.0167)} = \sqrt{\frac{4.5}{(0.0167)^2}} = \sqrt{4.5} \cdot \frac{1}{0.0167} = 127.28 \ \frac{CFU}{m^2}$$

$$\sqrt{R(\alpha,\beta)_{Bayes}} = \sqrt{\frac{\alpha}{\beta \cdot (e+\beta)}} < \sqrt{\frac{\alpha}{2 \cdot \beta^2}} < \frac{127.28}{2} \ \frac{CFU}{m^2}; e > \beta, e > 0.0167,$$

$$swab\ exposure\ is\ 0.002, \frac{0.0167}{0.002} = 8.35\ swabs, \mathrm{e} > 8.35\ \mathrm{swabs} \sim 9\ \mathrm{swabs}$$

In general, in order to decrease the risk of an implied component by N times through sampling, $e > \beta(N-1)$

# Sampling Design for Sampled Components

$$\sqrt{R(\alpha,\beta)_{Bayes}} = \sqrt{\frac{\alpha}{\beta\cdot(e+\beta)}} = C; e = \sqrt{\beta\cdot(\frac{\alpha}{\beta^2\cdot C} - 1)},$$

$$\alpha\text{=}1.7778, \beta = 0.0593, \mathrm{C} = 20\ \frac{CFU}{m^2}$$

$$e = 0.1251\ m^2, swab\ exposure\ is\ 0.002, \frac{0.1251}{0.002} = 62.55\ swabs, \mathrm{e}{\sim}63\ \mathrm{swabs}$$

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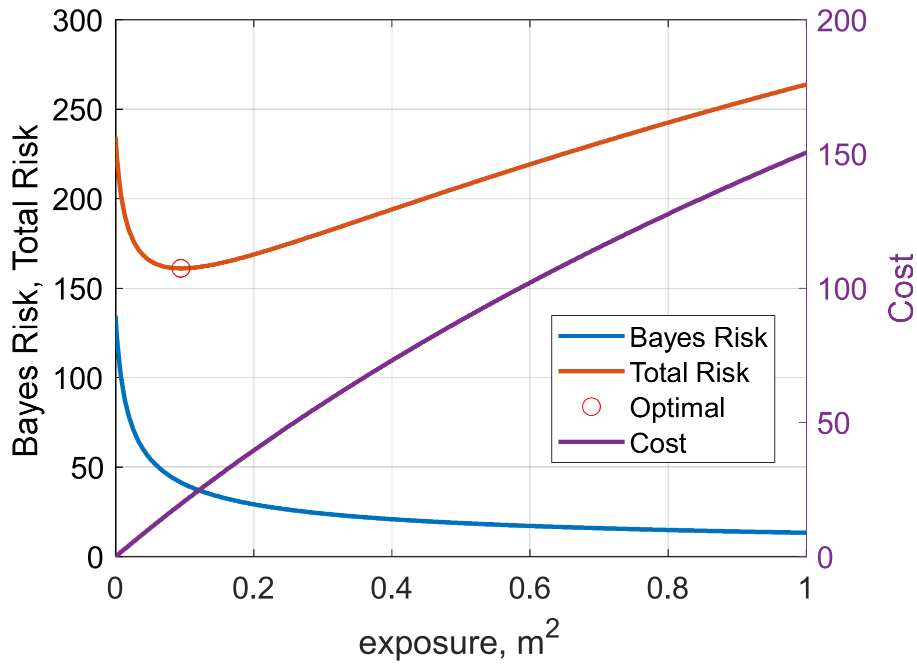
# Total Risk

$$TR_{Bayes}\,(\alpha,\beta,e) = \underbrace{R(\alpha,\beta,e)_{Bayes}}_{Uncertainty} + \underbrace{S_0(e) + e\cdot S}_{Cost} = \frac{\alpha}{\beta\cdot(e+\beta)} + S_0(e) + S * log_{10}(e)$$

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# Analysis of InSight's Implied Components

| Implied component | Implied from component | Implied Bioburden density, $\hat{\lambda}$, CFU/m$^2$ | Implied Risk, CFUs/m$^2$ | Total surface area of the implied component, m$^2$ | Optimal sampling area , m$^2$ | Optimal Risk, CFUs/m$^2$ | Optimal Cost, Units |
|---|---|---|---|---|---|---|---|
| 'Component 2' | 'Component 10' | 12.04819 | 17.03872 | 0.256 | 0.033779 | 12.65098 | 2.885537 |
| 'Component 106' | 'Component 108' | 13.51351 | 19.11099 | 0.533 | 0.0416 | 13.11212 | 3.54019 |
| 'Component 133' | 'Component 131' | 5.102041 | 4.165799 | 0.01298 | 6.61E-05 | 4.165331 | 0.005742 |
| 'Component 216' | 'Component 211' | 5.319149 | 7.522413 | 0.00625 | 6.61E-05 | 7.519769 | 0.005742 |
| 'Component 215' | 'Component 219' | 9.588831 | 13.56065 | 0.01922 | 0.016842 | 11.78968 | 1.450702 |
| 'Component 239' | 'Component 238' | 125.0000 | 176.7767 | 0.0024 | 0.0024 | 139.7542 | 0.208212 |
| 'Component 254' | 'Component 242' | 15.62500 | 22.09709 | 0.002 | 0.002 | 21.43732 | 0.173544 |
| 'Component 20' | 'Component 26' | 27.55906 | 14.73093 | 0.1736 | 6.61E-05 | 14.7271 | 0.005742 |
| 'Component 29' | 'Component 32' | 104.16670 | 65.88078 | 0.166 | 0.141017 | 25.12461 | 11.45846 |
| 'Component 36' | 'Component 38' | 15.49907 | 4.383799 | 2.0 | 6.61E-05 | 4.383619 | 0.005742 |
| 'Component 48' | 'Component 49' | 46.8750 | 38.27328 | 0.032 | 0.032 | 27.06329 | 2.735939 |

# Analysis of InSight's Sampled Components

| Component | Bioburden density, $\hat{\lambda}$, CFU/m$^2$ | Risk, CFUs/m$^2$ | Total surface area m$^2$ | Area sampled, m$^2$ | Optimal additional sampling area , m$^2$ | Optimal Risk, CFUs/m$^2$ | Optimal Cost, Units |
|---|---|---|---|---|---|---|---|
| 'Component 233' | 31.25 | 44.19417 | 0.0285 | 0.02 | 0.0285 | 26.49995 | 2.440859 |
| 'Component 236' | 173.0769 | 81.58924 | 0.5 | 0.0325 | 0.173103 | 29.48362 | 13.86722 |
| 'Component 237' | 93.7500 | 76.54655 | 0.5 | 0.02 | 0.143562 | 24.23936 | 11.65193 |
| 'Component 238' | 125.000 | 176.7767 | 0.0179 | 0.005 | 0.0179 | 75.54974 | 1.541023 |
| 'Component 242' | 15.625 | 22.09709 | 0.298 | 0.04 | 0.051017 | 13.71915 | 4.321927 |
| 'Component 243' | 48.24561 | 20.572 | 0.298 | 0.28 | 0.003169 | 20.2919 | 0.27481 |
| 'Component 245' | 35.71429 | 50.50763 | 0.282 | 0.0175 | 0.098621 | 17.80783 | 8.169593 |
| 'Component 246' | 62.5 | 88.38835 | 0.237 | 0.01 | 0.130309 | 21.25761 | 10.63945 |
| 'Component 26' | 27.55906 | 14.73093 | 0.454 | 0.255 | 6.61E-05 | 14.7271 | 0.005742 |
| 'Component 46' | 83.33333 | 117.8511 | 0.024 | 0.0075 | 0.024 | 52.70463 | 2.059991 |
| 'Component 49' | 46.875 | 38.27328 | 0.26 | 0.04 | 0.090713 | 19.54457 | 7.542059 |

# Recovery Efficiency (RE) and Measurement's noise (systematic and random errors)

*x-CFU counts*
*λ- bioburden density, CFUs/m²*
*e- exposure, pour ratio*area sampled, m²*

$$P(X=x|\lambda_{true}) = \frac{(\lambda_{true}\cdot e)^x}{x!} e^{-\lambda_{true}\cdot e},$$
$$x = 0,1,2,\dots, \lambda_{true} \in (0,\infty), e \in (0,\infty)$$

x=1,1,1,1,1

$$C_r^n p^r (1-p)^{n-r}$$

q → q·x;1,1

$$P(X=x|q\cdot\lambda_{true}) = \frac{(q\cdot\lambda_{true}\cdot e)^x}{x!} e^{-q\cdot\lambda_{true}\cdot e},$$

p → p·x;1,1,1

$$P(X=x|p\cdot\lambda_{true}) = \frac{(p\cdot\lambda_{true}\cdot e)^x}{x!} e^{-p\cdot\lambda_{true}\cdot e},$$

$$\hat{\lambda}_{MLE}^{PR} = \frac{x+alfa}{e+beta}, assumes\ perfect\ recovery, \text{(Perfect Recovery (PR) estimator)}$$

$$\hat{\lambda}_{MLE}^{RE} = \frac{x-\epsilon+alfa}{e+beta}, = \frac{x}{e}\cdot p, assumes\ partial\ recovery, (Recovery\ Efficiency(RE)\ estimator)$$

$$\hat{\lambda}_0 = 0, assumes\ no\ recovery, (Zero\ estimator)$$

p-probability of keeping a CFU count (efficiency)
q=(1-p)-probability of deleting a CFU count (1-efficiency)

$$Risk = MSE = E\left[(\hat{\lambda}-\lambda_{true})^2\right], \boldsymbol{Symmetric}\ Mean\ Squared\ Error\ (MSE)$$

# Bias and Variance of the RE estimator

$$E\left[\hat{\lambda}_{MLE}^{RE}\right] = E\left[\frac{x-\varepsilon}{e}\right] = \frac{1}{e}E[x-\varepsilon] = \frac{1}{e}\cdot(\lambda_{true}\cdot\varepsilon) - E(\varepsilon) = \lambda_{true} - \lambda_{true}\cdot \mathrm{q} = \lambda_{true}\cdot(1-\mathrm{q}) = \lambda_{true}\cdot p$$

$$Bias\left[\hat{\lambda}_{MLE}^{RE}\right] = \lambda_{true} - \lambda_{true}\cdot \mathrm{q} - \lambda_{true} = -\boldsymbol{\lambda_{true}}\cdot \mathbf{q}$$

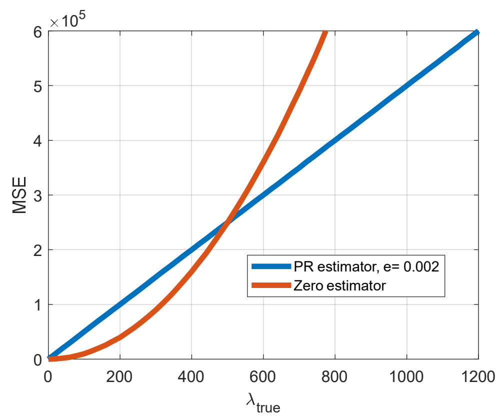
$$Var\left[\hat{\lambda}_{MLE}^{RE}\right] = Var\left[\frac{x-\epsilon}{e}\right] = \frac{1}{e^2}Var[x-\epsilon] = Var\left[\frac{x}{e}\right] + Var\left[\frac{\epsilon}{e}\right] - 2\cdot Cov\left(\frac{x}{e},\frac{\varepsilon}{e}\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(E\left[\frac{x}{e}\cdot\frac{q\cdot x}{e}\right] - E\left[\frac{x}{e}\right]\cdot E\left[\frac{q\cdot x}{e}\right]\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(q\cdot E\left[\frac{x}{e}\cdot\frac{x}{e}\right] - q\cdot E\left[\frac{x}{e}\right]\cdot E\left[\frac{x}{e}\right]\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(q\cdot E\left[\left(\frac{x}{e}\right)^2\right] - q\cdot\left(E\left[\frac{x}{e}\right]\right)^2\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\left(E\left[\left(\frac{x}{e}\right)^2\right] - \left(E\left[\frac{x}{e}\right]\right)^2\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\cdot Var\left[\frac{x}{e}\right] = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\cdot\frac{\lambda_{true}}{e} = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1} + q^2 - \mathbf{2}\cdot\boldsymbol{q}) = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot\boldsymbol{p}^{\mathbf{2}}$$

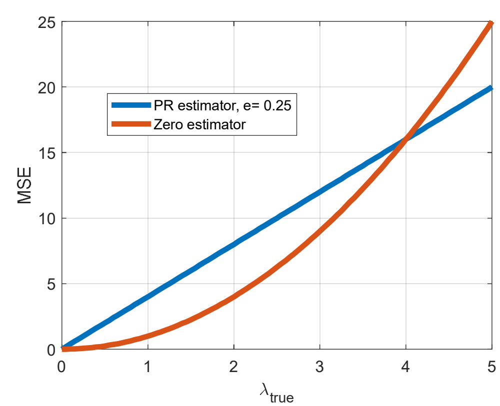
$$MSE\left(\hat{\lambda}_{MLE}^{RE}\right) = Bias^2 + Var = (-\boldsymbol{\lambda_{true}}\cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = (-\boldsymbol{\lambda_{true}}\cdot(\mathbf{1}-\boldsymbol{p}))^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot\boldsymbol{p}^{\mathbf{2}}$$

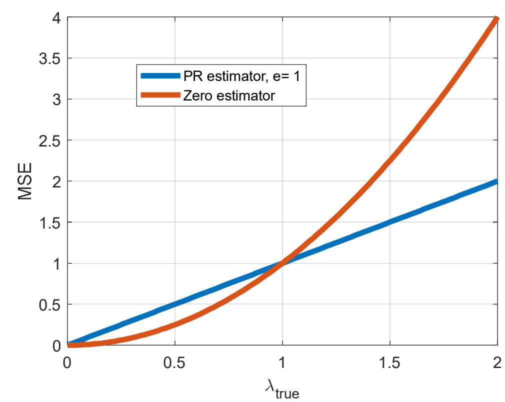
# MSE of the Recover Efficiency for Symmetric Penalty Function

$$MSE(\hat{\lambda}_{MLE}^{RE}) = Bias^2 + Var = (-\lambda_{true} \cdot q)^2 + \frac{\lambda_{true}}{e} \cdot (1-q)^2 = (-\lambda_{true} \cdot (1-p))^2 + \frac{\lambda_{true}}{e} \cdot p^2$$

$$MSE(\hat{\lambda}_{MLE}^{PR}) = \frac{\lambda_{true}}{e}, p = 1 \qquad MSE_0 = \lambda_{true}{}^2, p = 0 \qquad \lambda_{true} < \frac{1}{e}$$




Zero estimator (p=0) will dominate PR estimator (p=1) up to the values of $\lambda_{true}$ <1/e

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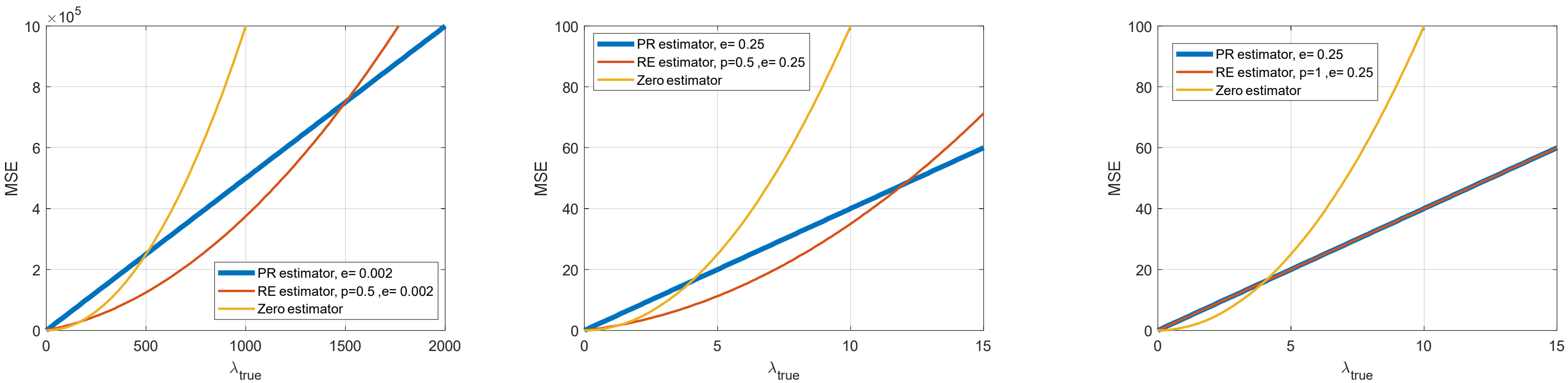
# MSE of the Recovery Efficiency Model as a Function of $\lambda_{true}$

$$MSE\left(\hat{\lambda}_{MLE}^{RE}\right) = Bias^2 + Var = (-\boldsymbol{\lambda}_{true}\cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda}_{true}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = (-\boldsymbol{\lambda}_{true}\cdot(\mathbf{1}-\boldsymbol{p}))^2 + \frac{\lambda_{true}}{e}\cdot \boldsymbol{p}^{\mathbf{2}}$$




RE estimator (0<p<1) will dominate PR estimator (p=1) up to the values of $\lambda_{true} < \frac{(1-p)}{e\cdot(1-p)}$, RE estimator will dominate Zero estimator (p=0) for $\lambda_{true} > \frac{p}{e\cdot(2-p)}$ . In addition, for $\lambda_{true} < \frac{p}{e\cdot(2-p)}$ , Zero estimator will dominate both RE and PR estimator

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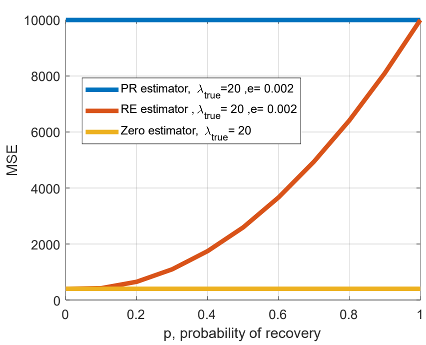
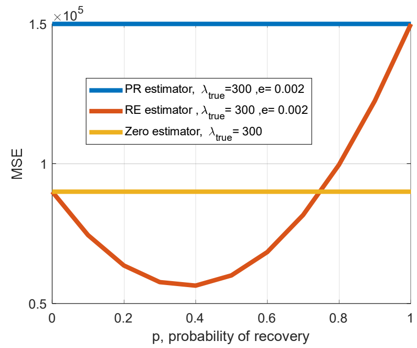
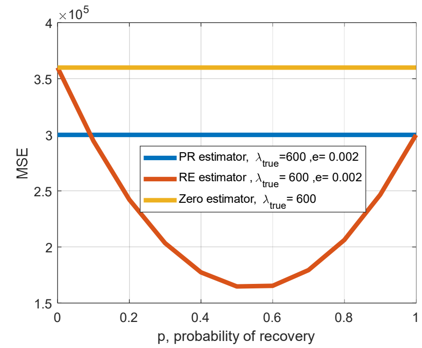
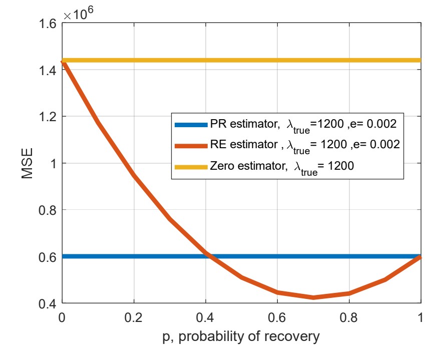
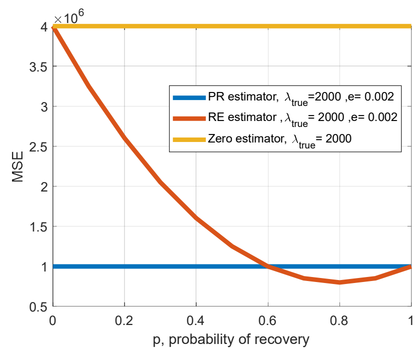
# MSE of the Recovery Efficiency Model as a Function of p for swab exposure




$$MSE(\hat{\lambda}^{RE}_{MLE}) = Bias^2 + Var = (-\boldsymbol{\lambda}_{true}\cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda}_{true}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q}) = (-\boldsymbol{\lambda}_{true}\cdot(\mathbf{1}-\boldsymbol{p}))^2 + \frac{\lambda_{true}}{e}\cdot \boldsymbol{p}^2$$

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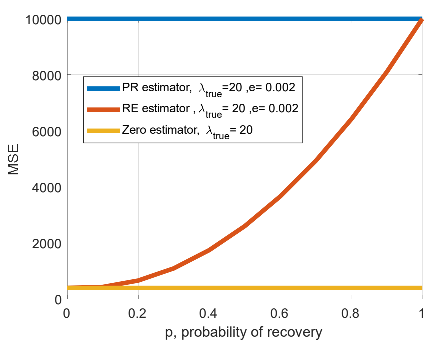
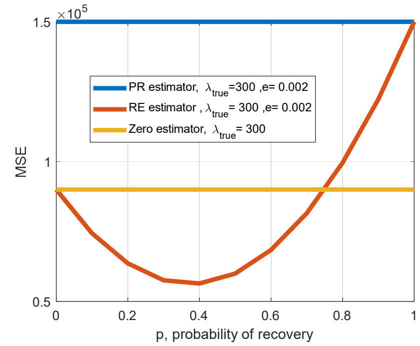
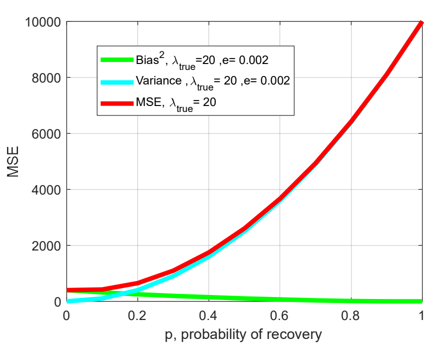
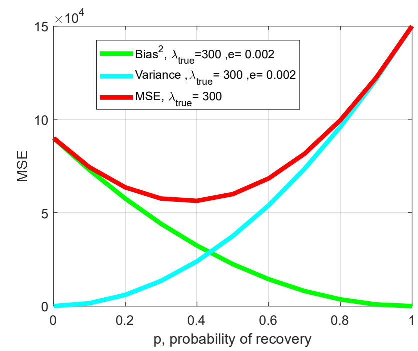
# Bias-Variance Decomposition of the RE estimator



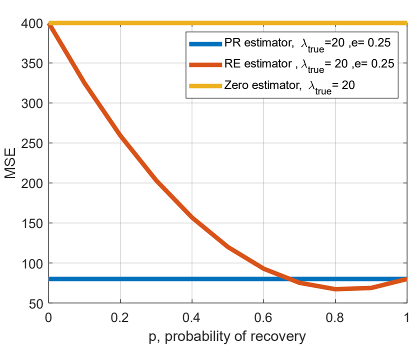

$$\hat{\lambda}_{MLE}^{PR} = \frac{1}{0.002} = 500\ CFUs/m^2$$

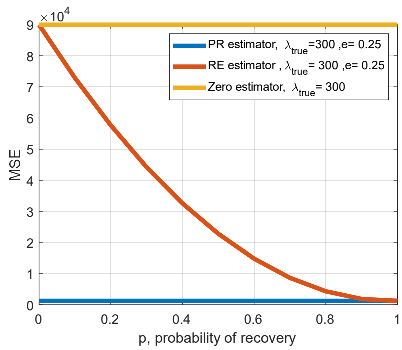


# MSE of the Recovery Efficiency Model as a Function of p for wipe exposure




$$MSE(\hat{\lambda}_{MLE}^{RE}) = (-\boldsymbol{\lambda_{true}} \cdot (\mathbf{1} - \boldsymbol{p}))^2 + \frac{\lambda_{true}}{e} \cdot \boldsymbol{p^2}$$

- The RE estimator is a compromise between perfect recovery estimator and zero estimator
- RE estimator (0<p<1) will dominate PR estimator (RE=1,p=1) up to the values of $\lambda_{true} < \frac{(1-p)}{e \cdot (1-p)}$
- The degree of domination is a function of p and e
- For small e=0.002 (swab), and small $\lambda_{true}$ , the domination is guaranteed for any value of efficiency p.
- As $\lambda_{true}$ increases, $MSE(\hat{\lambda}_{MLE}^{RE})$shows a minimal value which is reached for optimal p
- For further increase in $\lambda_{true}$ the optimal value still exists , however there a minimal value of p below which the RE estimator no longer dominates the PR estimator
- For large e≥0.25, the influence of recovery efficiency is significantly more prominent (decisive actually) as even for small $\lambda_{true}$ , the efficiency needs to be nearly 1 to approach the PR estimator
- The RE estimator performs as a shrinkage estimator, as it shrinks variance of the estimate at the expense of introducing bias
- This may lead to a better estimate that the perfect recovery estimator

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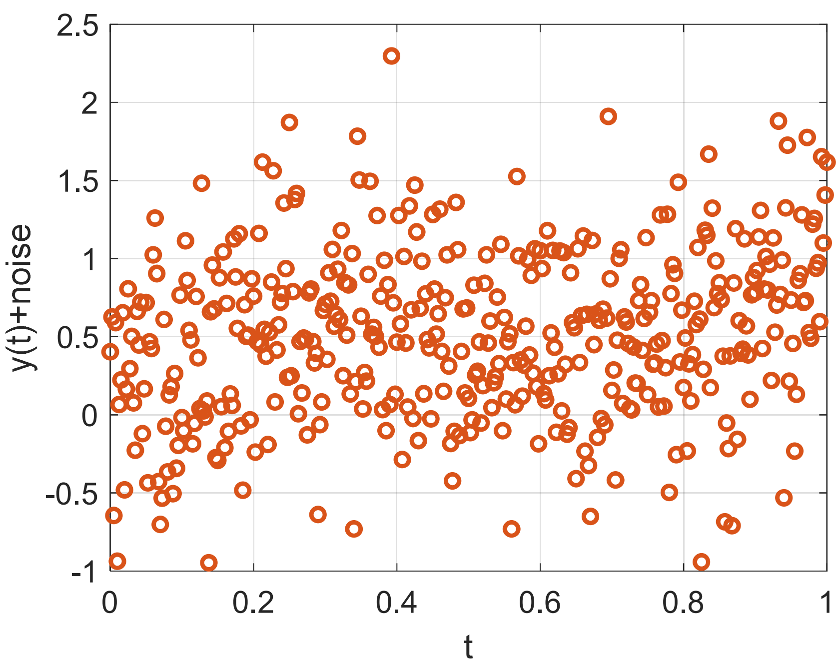
# Learning from Noisy Data

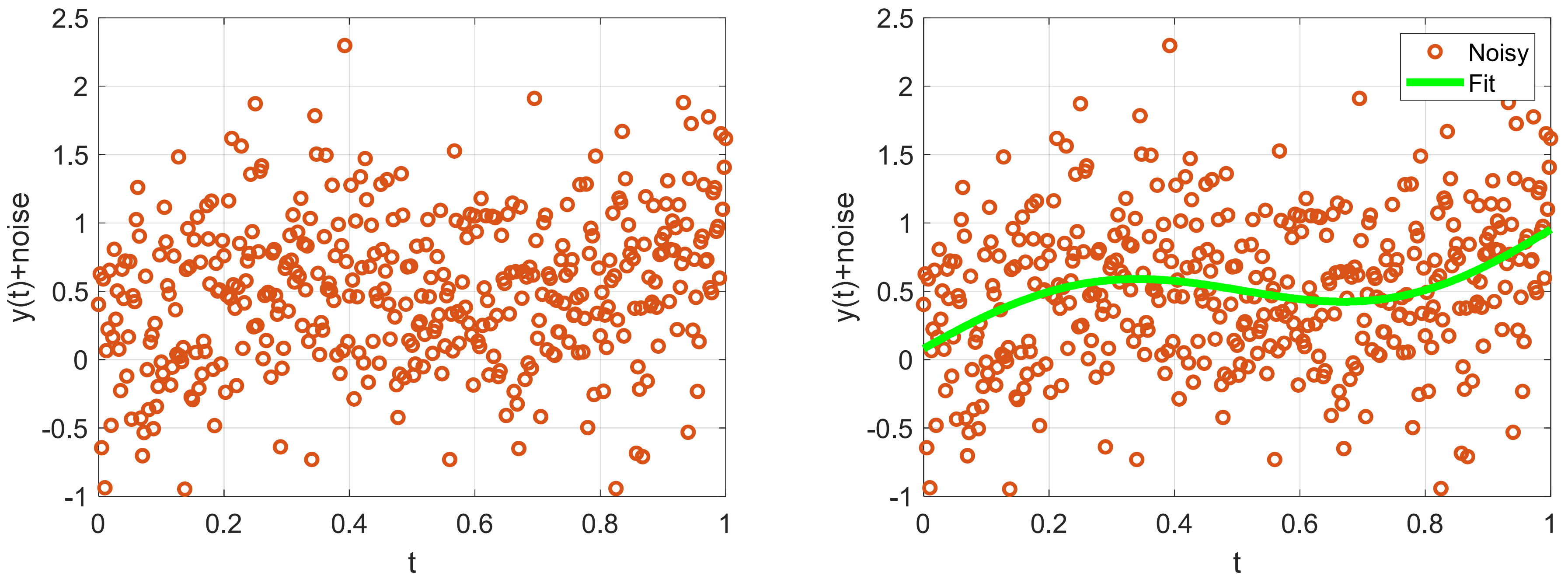



In 1923, the French mathematician Hadamard introduced the notion of well-posed problems.

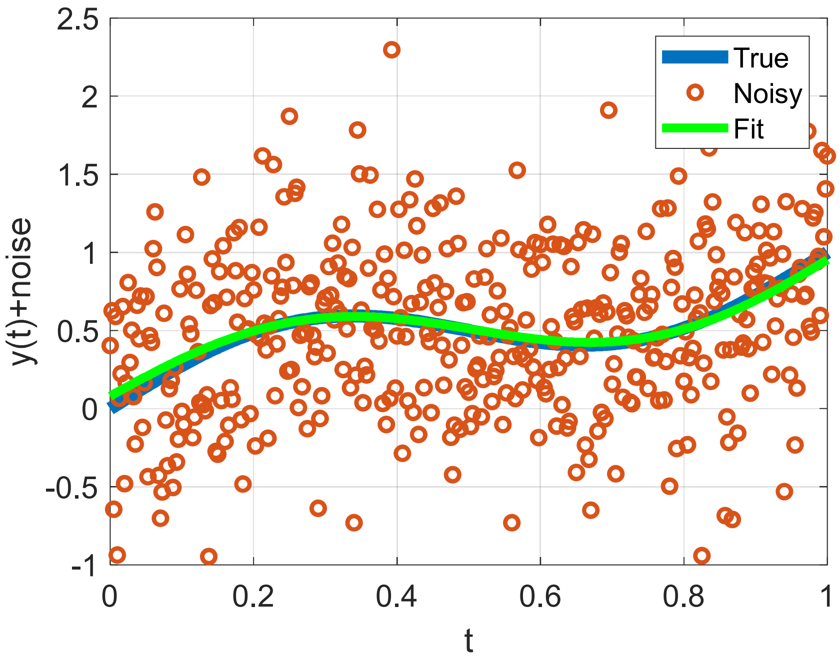
According to Hadamard, a problem is called well-posed iff:

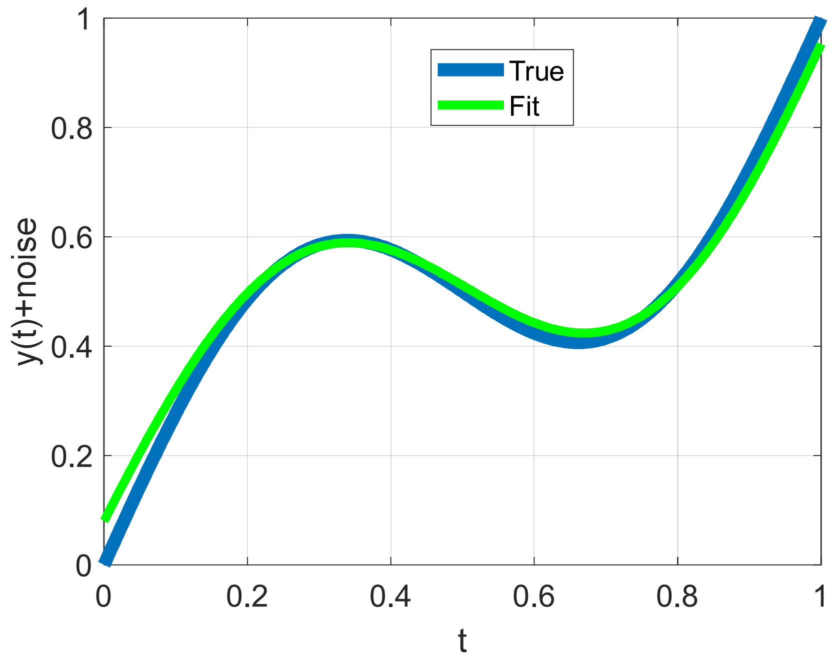
1. A solution to the problem exists (existence).
2. This solution is unique (uniqueness).
3. This unique solution is stable under small perturbations in the data, in other words small perturbations in the data should cause small perturbations in the solution (stability).

# Learning from Noisy Data

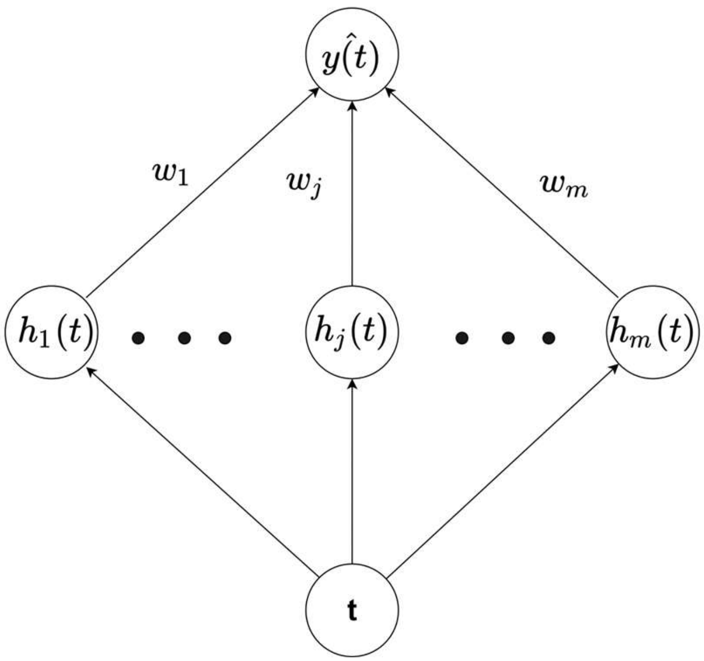


# Learning from Noisy Data



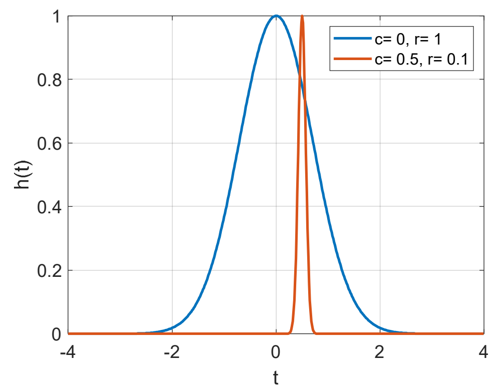
# Radial Basis Function Network and Regularization




$$\hat{y}(t_1) = w_1 \cdot h_1(t_1) + w_2 \cdot h_2(t_1) + \cdots w_m \cdot h_m(t_1)$$
$$\hat{y}(t_2) = w_1 \cdot h_1(t_2) + w_2 \cdot h_2(t_2) + \cdots w_m \cdot h_m(t_2)$$
$$\vdots$$
$$\hat{y}(t_p) = w_1 \cdot h_1(t_p) + w_2 \cdot h_2(t_p) + \cdots w_m \cdot h_m(t_p)$$

$$\hat{y}(t) = \sum_{j=1}^{m} w_j \cdot h_j(t)$$

$$\underbrace{\hat{y}}_{px1} = \underbrace{H}_{pxm} \cdot \underbrace{w}_{mx1}$$




$$h(t) = e^{\left(-\frac{(t-c)^2}{r^2}\right)}$$

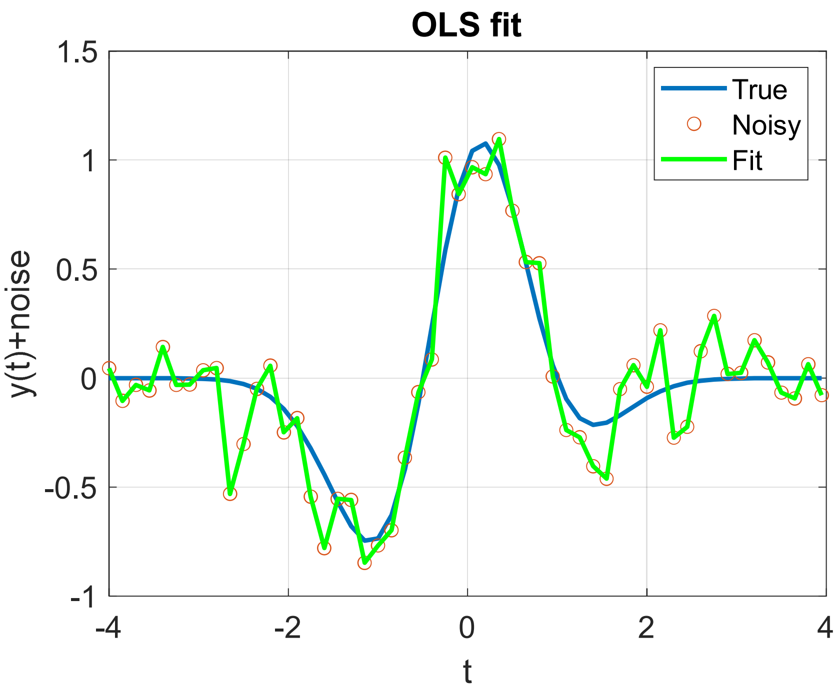
# Ordinary Least Squares

$$E = \sum_{i=1}^{p} (\hat{y}(t_i) - \tilde{y}_i)^2 = (\tilde{y} - H \cdot w)^T \cdot (\tilde{y} - H \cdot w)$$

$$w = (H^T \cdot H)^{-1} H^T \cdot \tilde{y}$$

$$\hat{y}(t) = \sum_{j=1}^{m} w_j \cdot h_j(t)$$

$$\{(t_i, \tilde{y}_i)\}_{i=1}^{p}$$



# Regularized Least Squares and Generalized Cross-Validation (GCV)

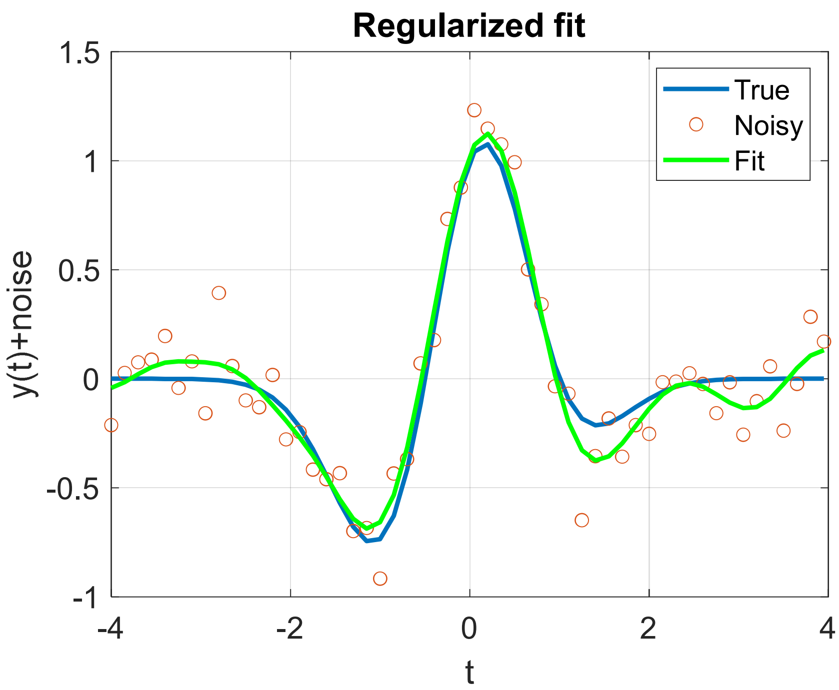
$$E = \sum_{i=1}^{p} (\hat{y}(t_i) - \tilde{y}_i)^2 + \mu \cdot \sum_{j=1}^{m} w_j^2 = (\tilde{y} - H \cdot w)^T \cdot (\tilde{y} - H \cdot w) + \mu \cdot w^T \cdot w$$

$$w_\mu = (H^T \cdot H + \mu \cdot I_m)^{-1} H^T \cdot \tilde{y}$$

$$\underbrace{\hat{y}}_{px1} = \underbrace{H}_{pxm} \cdot \underbrace{(H^T \cdot H + \mu \cdot I)^{-1} H^T \cdot \tilde{y}}_{mx1} = A_\mu \cdot \tilde{y}$$

$$A_\mu = H \cdot (H^T \cdot H + \mu \cdot I)^{-1} H^T$$

$$GCV(\mu) = \frac{\left\| H \cdot w_\mu - \tilde{y} \right\|^2}{\left(m - trace(A_\mu)\right)^2}$$

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# The Problem of Differentiation

$$g(x) = f(x) + a \cdot \sin(\omega \cdot x)\,;\, g'(x) = f'(x) + \omega \cdot a \cdot \cos(\omega \cdot x)$$

$$g'(x) - f'(x) = \omega \cdot a \cdot \cos(\omega \cdot x)$$

$$G(x) = \int f(x)dx - \frac{a}{w} \cdot \cos(w \cdot x) + C$$

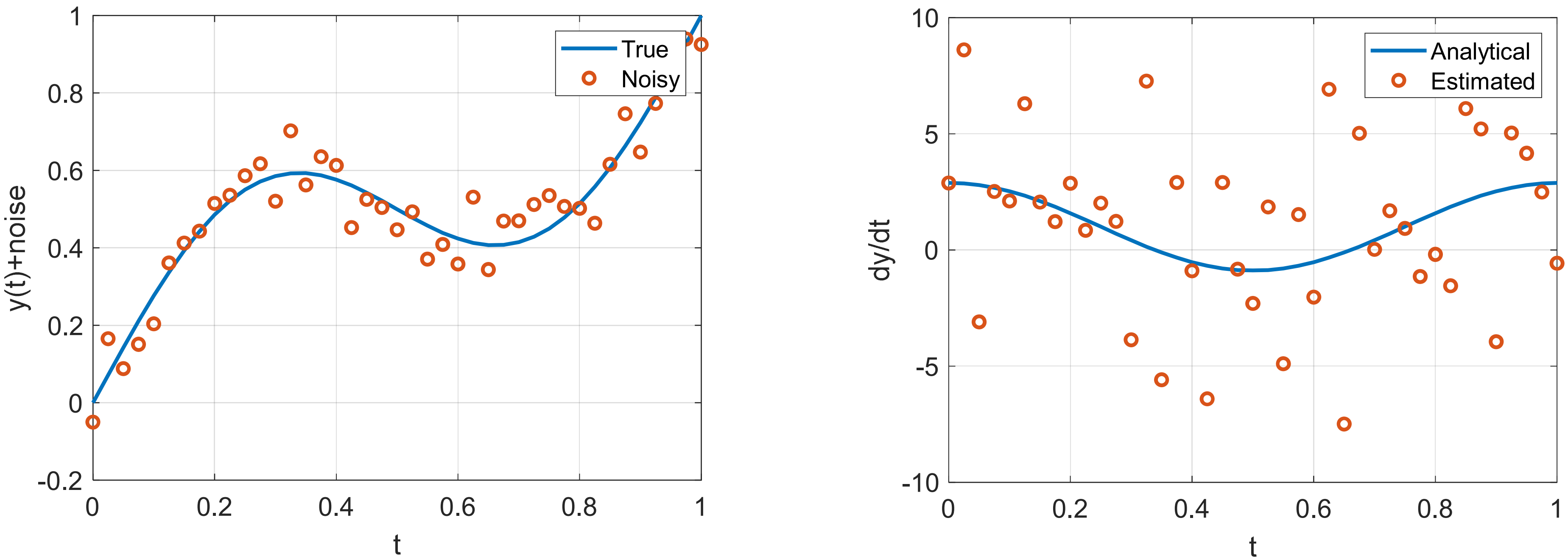
$$G(x) - \int f(x)dx = C - \frac{a}{w} \cdot \cos(w \cdot x)$$

$$F(x) + \varepsilon = \int_0^x F'(t)dt, \qquad F(0) = 0$$

$$\frac{d[F(x)+\varepsilon]}{dx} = \frac{d}{dx}\int_0^x F'(t)dt = F'(x) + \frac{d\varepsilon}{dx}$$

# Naïve Differentiation of the Sampled Data

$$y(t) = t + 0.3 \cdot \sin(2\pi \cdot t) + \varepsilon;\ \bar{\varepsilon} = 0; \sigma_{\varepsilon} = 0.05; \sigma_{Residuals} = 3.6; \frac{\sigma_{Residuals}}{\sigma_{\varepsilon}} = 72$$




$$y'(t_1) = \frac{y(t_2) - y(t_1)}{t_2 - t_1}, y'(t_2) = \frac{y(t_3) - y(t_2)}{t_3 - t_2}, \ldots, y'(t_{n-1}) = \frac{y(t_n) - y(t_{n-1})}{t_n - t_{n-1}}$$

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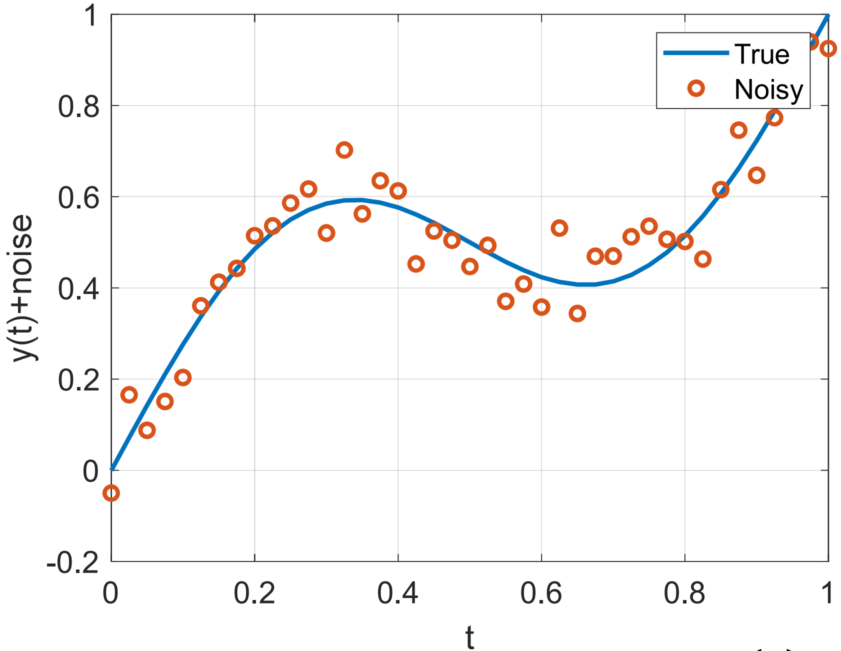
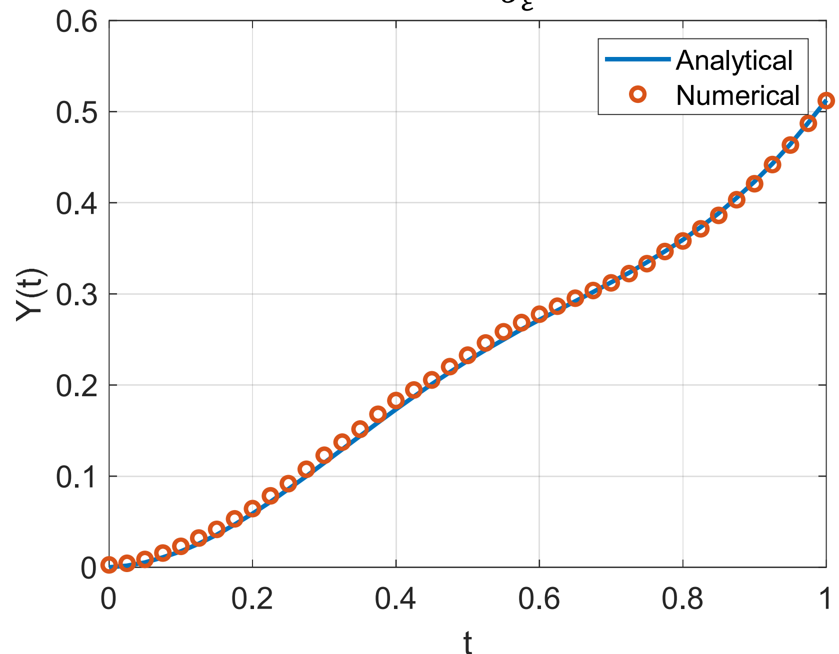
# Integration of the Noisy Data

$$y(t) = t + 0.3 \cdot \sin(2\pi \cdot t) + \varepsilon;\ \bar{\varepsilon} = 0, \sigma_\varepsilon = 0.05; \sigma_{Residuals} = 0.004; \frac{\sigma_{Residuals}}{\sigma_\varepsilon} = 0.08$$




$$S(n) = \sum_{i=1}^{n} y(t_i) \cdot \Delta t, \Delta t = t_i - t_{i-1}$$

$$S(1) = y(t_1) \cdot \Delta t; S(2) = [y(t_1) + y(t_2)] \cdot \Delta t; S(n) = [y(t_1) + y(t_2) + \cdots + y(t_n)] \cdot \Delta t$$

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# Frequency Response of Integration and Differentiation

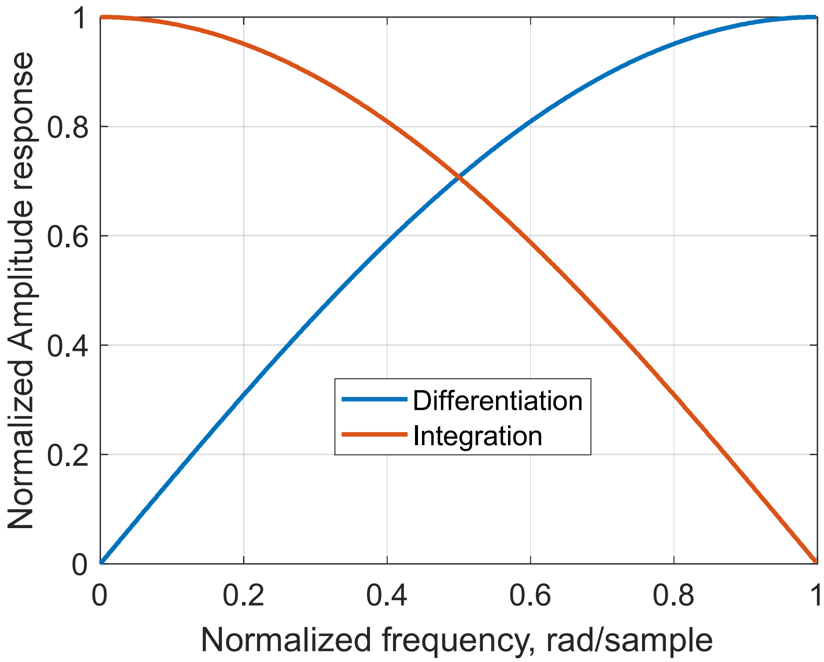
$$y'(t_1) = \frac{y(t_2) - y(t_1)}{t_2 - t_1} = [y(t_2) - y(t_1)] \cdot \frac{1}{\Delta t}; \Delta t = t_2 - t_1$$

$$h_{diff} = [1 \;\; -1], \Delta t = 1$$

$$S = [y(t_1) + y(t_2)] \cdot \Delta t$$

$$h_{int} = [1 \;\; 1], \Delta t = 1$$

Amplitude response is the absolute value of the Fourier transform of the filter's coefficients (impulse response).

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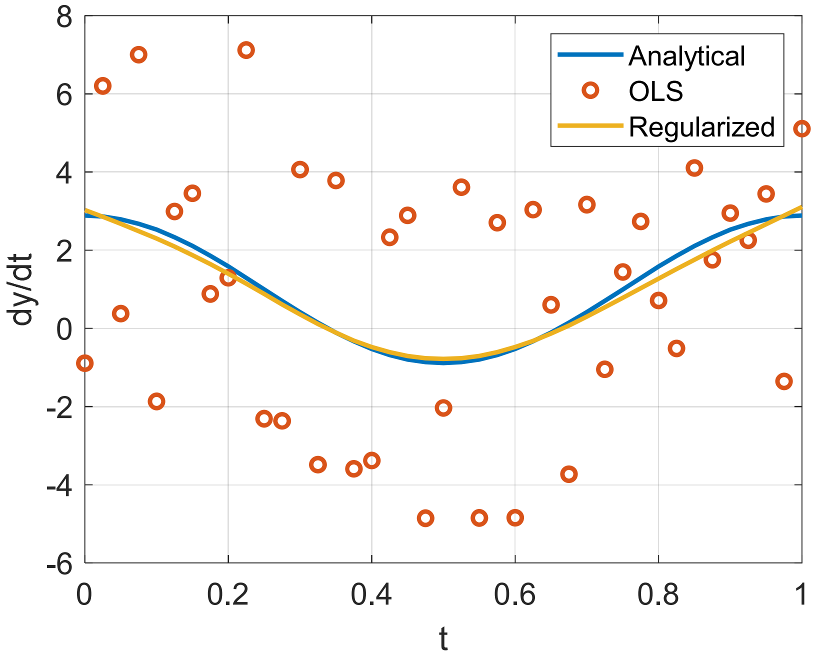
# Regularized vs Naïve Derivatives




$$\underbrace{A}_{nxn} = \underbrace{U}_{nxn} \cdot \underbrace{\Sigma}_{nxn} \cdot \underbrace{V}_{nxn}^{T} \qquad \|S - A \cdot y\|^2 \rightarrow min$$

$$\hat{y}_{OL} = V \cdot \Sigma^{-1} \cdot U^T \cdot S = \sum_{i=1}^{N} \frac{u_i^T \cdot S}{\sigma_i} \cdot v_i$$

$$\|S - A \cdot y\|^2 + \lambda \cdot \|L \cdot \hat{y}\|^2 \rightarrow min$$

$$\hat{\lambda}_{Reg} = [A^T \cdot A + \mu \cdot L^T \cdot L]^{-1} \cdot A^T \cdot S = V \cdot (\Sigma^2 + \mu \cdot L^T \cdot L)^{-1} \cdot \Sigma \cdot U^T \cdot S$$

$$= \sum_{i=1}^{N} f_i \frac{u_i^T \cdot S}{\sigma_i} \cdot v_i \qquad f_i = \frac{\sigma_i^2}{\sigma_i^2 + \mu}, i = 1, \ldots, N$$

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# Regularized Differentiation for Bio Density Estimation

$$\|S - A \cdot y\|^2 + \mu \cdot \|L \cdot \hat{y}\|^2 \rightarrow min$$

$$\hat{\lambda}_i^{MLE} = \frac{x_i}{E_i}, i = 1, \ldots n$$

$$\lambda_1 = \frac{S(1) - S(0)}{E_1} = \frac{1}{0.0020}; \lambda_2 = \frac{S(2) - S(1)}{E_2} = \frac{0}{0.0020}$$

$$\lambda_{13} = \frac{S(13) - S(12)}{E_{13}} = \frac{3}{0.0020}; \ldots; \lambda_{24} = \frac{S(24) - S(23)}{E_2} = \frac{14}{0.0020}$$

| Component 261 Sample No. | CFUs Observed | Area Sampled, $m^2$ | Pour Fraction | Exposure, $m^2$ | Cumulative CFU Count, S |
|---|---|---|---|---|---|
| 0 | | | | | 0 |
| 1 | 1 | 0.0025 | 0.8 | 0.0020 | 1 |
| 2 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 3 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 4 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 5 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 6 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 7 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 8 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 9 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 10 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 11 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 12 | 0 | 0.0025 | 0.8 | 0.0020 | 1 |
| 13 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 14 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 15 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 16 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 17 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 18 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 19 | 0 | 0.0025 | 0.8 | 0.0020 | 4 |
| 20 | 6 | 0.0025 | 0.8 | 0.0020 | 10 |
| 21 | 8 | 0.0025 | 0.8 | 0.0020 | 18 |
| 22 | 10 | 0.0025 | 0.8 | 0.0020 | 28 |
| 23 | 10 | 0.0025 | 0.8 | 0.0020 | 38 |
| 24 | 14 | 0.0025 | 0.8 | 0.0020 | 52 |
| Total | 52 | 0.0600 | 0.8 | 0.0480 | - |

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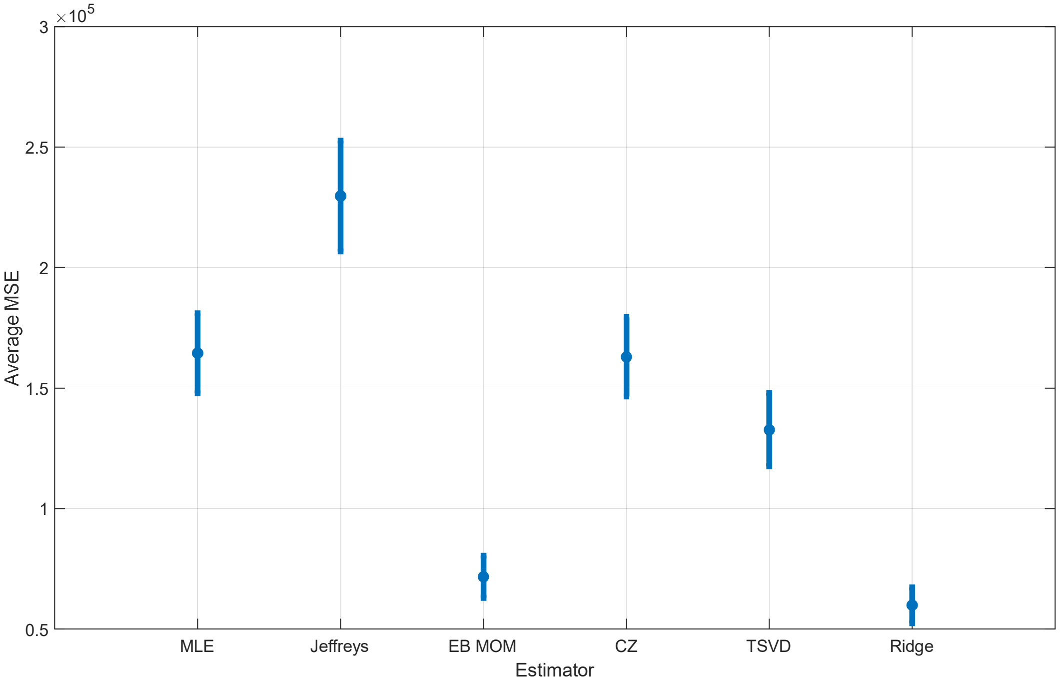


$$\hat{\lambda}_i(x_i) = \frac{x_i}{E_i} \qquad \hat{\lambda}_i(x_i) = \frac{x_i + 0.5}{E_i}$$

$$\hat{\lambda}_i(x_i) = \frac{x_i + \alpha_{MOM}}{E_i + \beta_{MOM}} \qquad \hat{\lambda}_{TSVD} = \sum_{i=1}^{k} \frac{u_i^T \cdot S}{\sigma_i} \cdot v_i$$

$$\hat{\lambda}_i^{CZ} = \frac{x_i}{E_i} - \frac{\gamma + N - 1}{\sum \frac{x_i}{E_i} + \gamma + N - 1} \cdot \left(\frac{x_i}{E_i}\right), i = 1, \ldots N$$

$$\hat{\lambda}_{Ridge} = \sum_{i=1}^{N} f_i \frac{u_i^T \cdot S}{\sigma_i} \cdot v_i$$

$$P(X = x | \lambda_{true}) = \frac{(\lambda_{true} \cdot E)^x}{x!} e^{-\lambda_{true} \cdot E}, x = 0,1,2, \ldots, \lambda_{true} \in (0, \infty), \text{E} \in (0, \infty)$$

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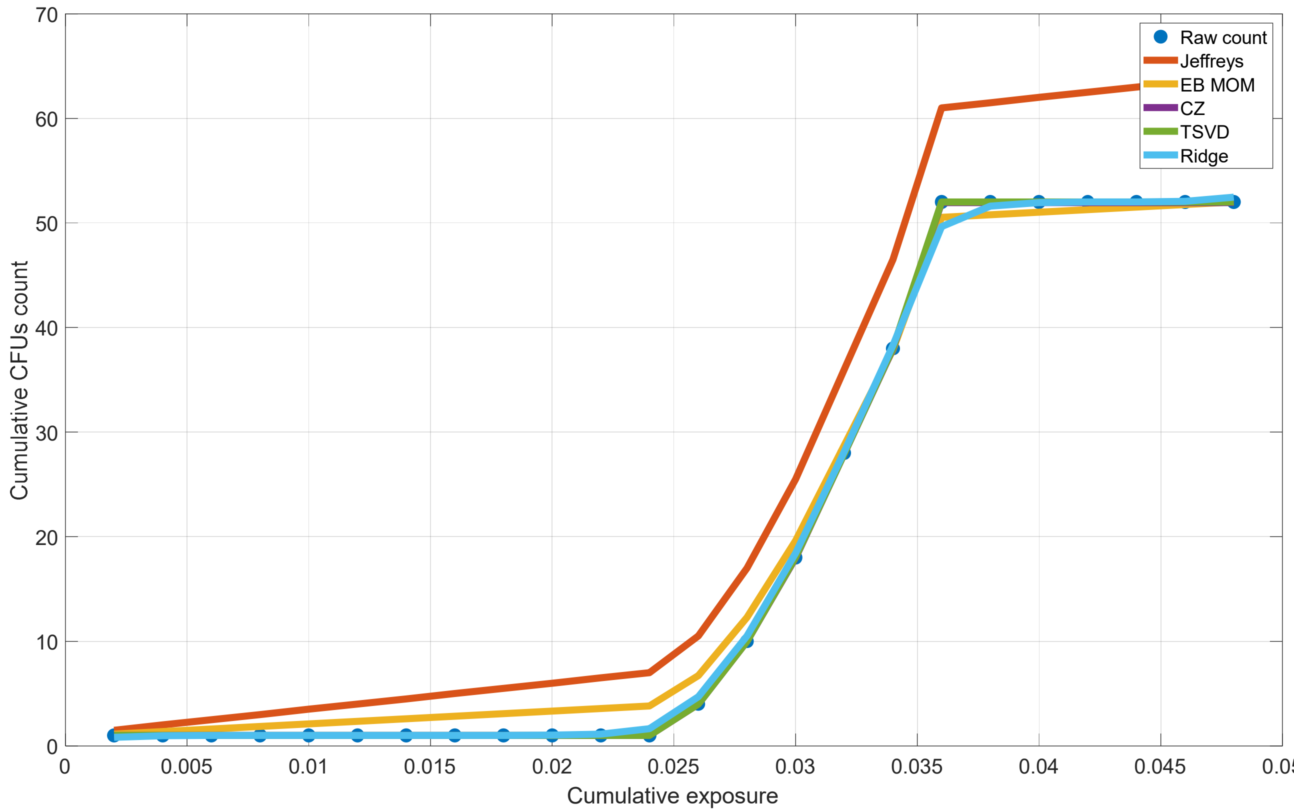
$$Gamma(\lambda_{true} | \alpha = 1.8, \beta = 0.001), \hat{\lambda} = 179.5$$

# Component 261

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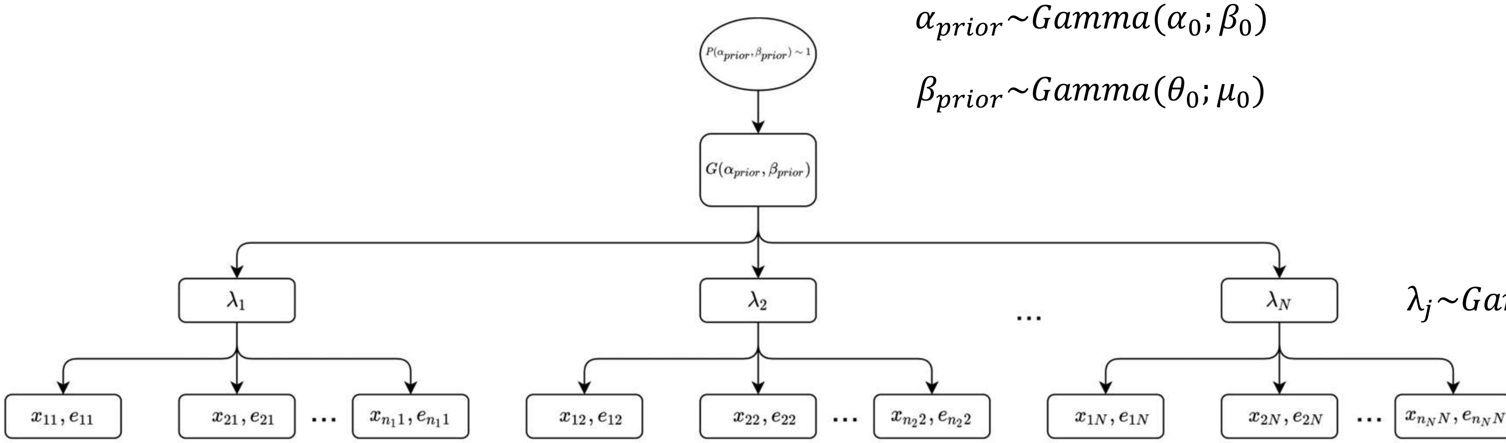
# Hierarchical Bayesian (HB) Approach

$\alpha_{prior} \sim Gamma(\alpha_0; \beta_0)$

$\beta_{prior} \sim Gamma(\theta_0; \mu_0)$




$\lambda_j \sim Gamma(\alpha_{prior}; \beta_{prior})$

$x_{ij} \sim Poisson(\lambda_j \cdot e_{i,j})$

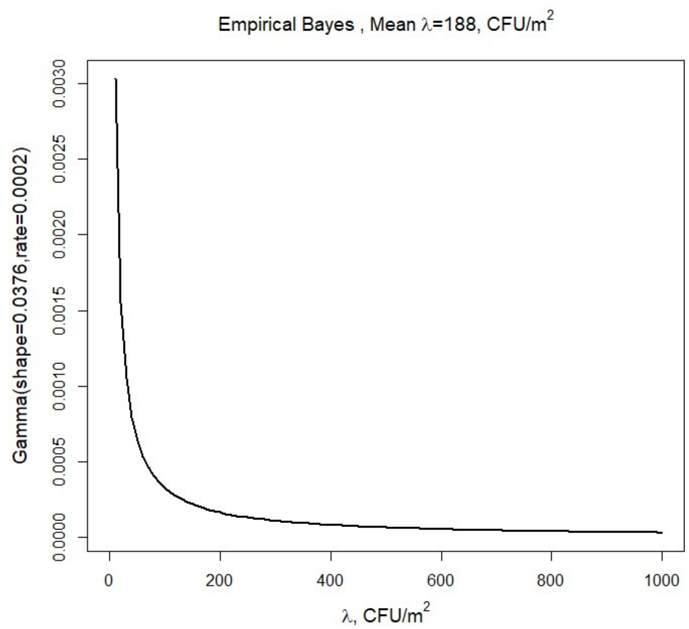
$j = 1 \ldots N - number\ of\ componets$

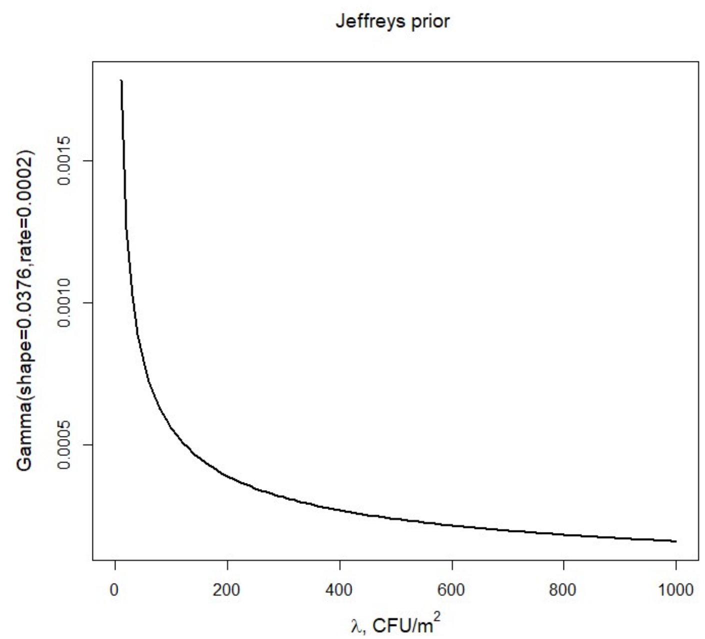
$i = 1 \ldots n_N - number\ of\ samples\ for\ Nth\ component$

# Summary of Bioburden Data for the Nine Components.

| Component | CFU Count | Area Sampled, $m^2$ | Exposure: Area Sampled*Pour Fraction, $m^2$ | Total Surface of the Component, $m^2$ | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|
| 9 | 0 | 0.6031 | 0.2167 | 0.7580 | 79.5650 |
| 73 | 0 | 2.4200 | 0.6160 | 2.7400 | 88.3212 |
| 300 | 1 | 2.6600 | 0.6705 | 5.0000 | 53.2000 |
| 169 | 1 | 0.2400 | 0.1920 | 0.5850 | 41.0260 |
| 283 | 5 | 4.5710 | 1.1427 | 12.0000 | 38.0920 |
| 243 | 5 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |
| 38 | 12 | 3.1050 | 0.8065 | 10.0000 | 31.0500 |
| 261 | 52 | 0.0600 | 0.0480 | 0.3120 | 19.2310 |
| 67 | 0 | 0.8575 | 0.2460 | 7.1500 | 11.9930 |

# Jeffreys prior vs Empirical Bayes (method of moments) vs Hierarchical Bayes

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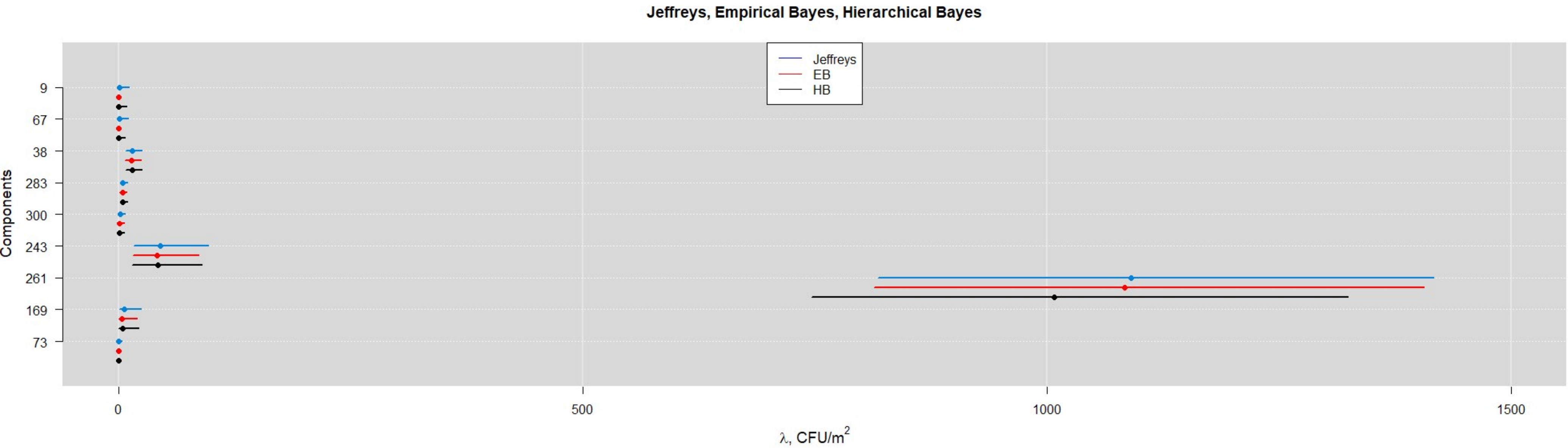
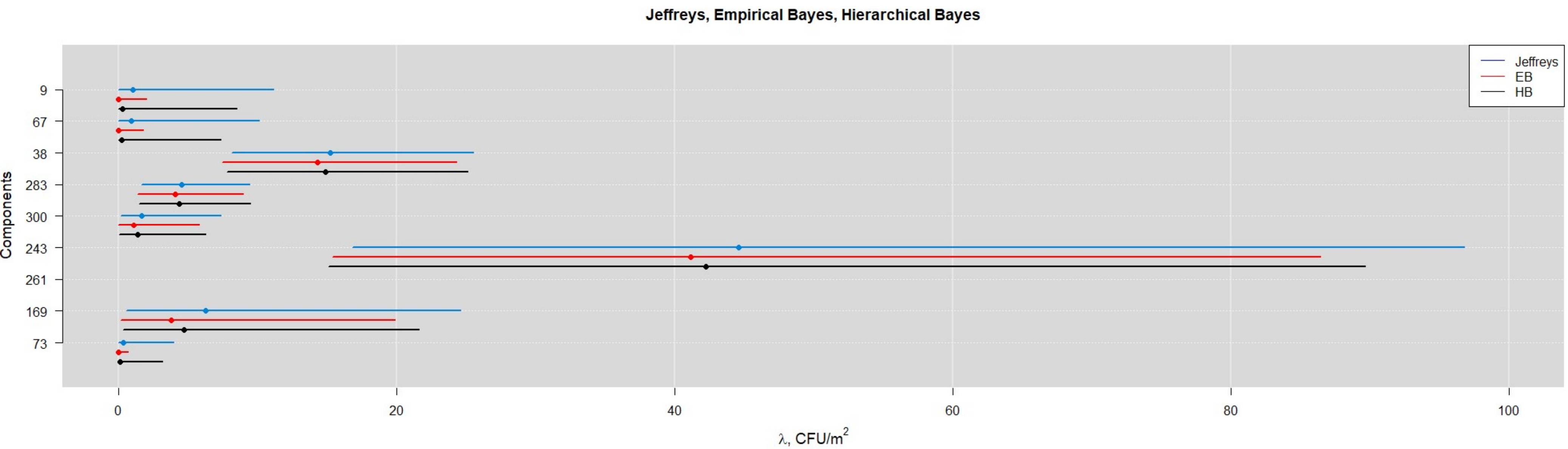
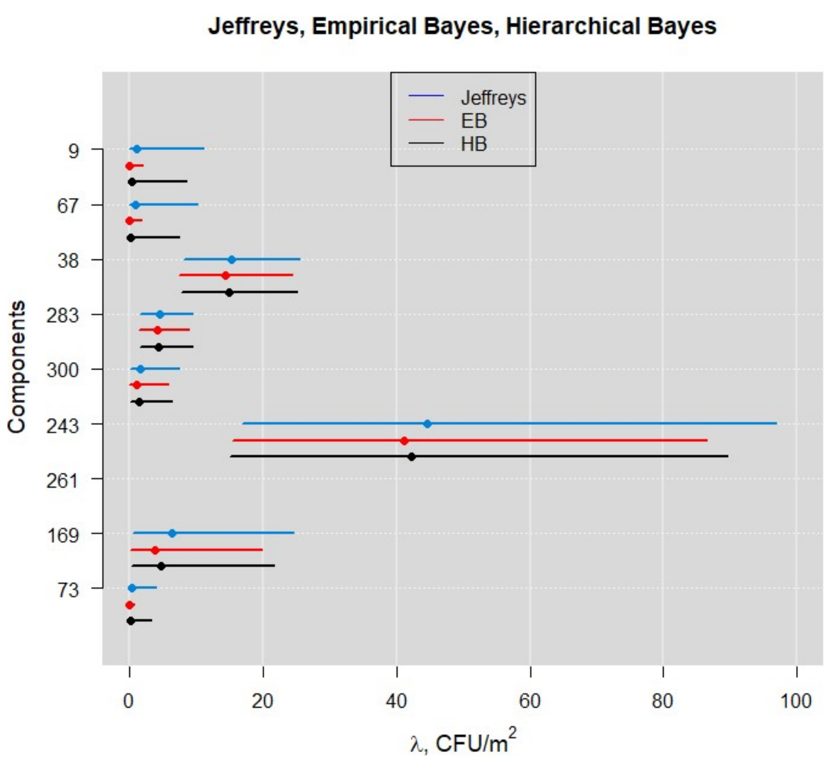
# Jeffreys prior vs Empirical Bayes (method of moments) vs Hierarchical Baves



# Jeffreys prior vs Empirical Bayes (method of moments) vs Hierarchical Bayes

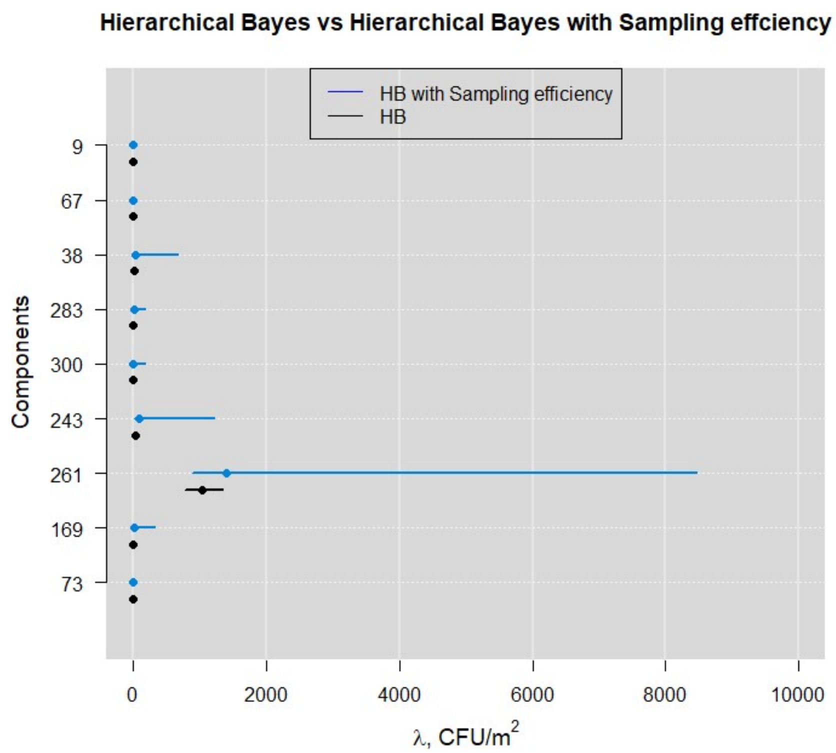


# Jeffreys prior vs Empirical Bayes (method of moments) vs Hierarchical Bayes



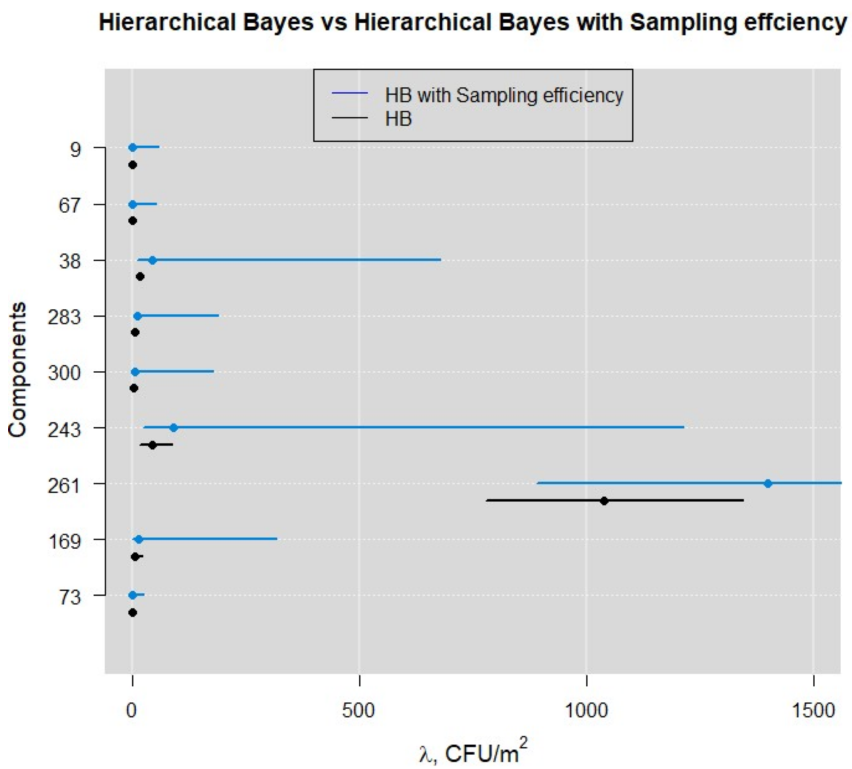

| Component | CFU Count | Area Sampled, m² | Exposure: Area Sampled*Pour Fraction, m² | Total Surface of the Component, m² | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|
| 9 | 0 | 0.6031 | 0.2167 | 0.7580 | 79.5650 |
| 67 | 0 | 0.8575 | 0.2460 | 7.1500 | 11.9930 |
| 38 | 12 | 3.1050 | 0.8065 | 10.0000 | 31.0500 |
| 283 | 5 | 4.5710 | 1.1427 | 12.0000 | 38.0920 |
| 300 | 1 | 2.6600 | 0.6705 | 5.0000 | 53.2000 |
| 243 | 5 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |
| 261 | 52 | 0.0600 | 0.0480 | 0.3120 | 19.2310 |
| 169 | 1 | 0.2400 | 0.1920 | 0.5850 | 41.0260 |
| 73 | 0 | 2.4200 | 0.6160 | 2.7400 | 88.3212 |

# Recovery Efficiency and Hierarchical Bayes

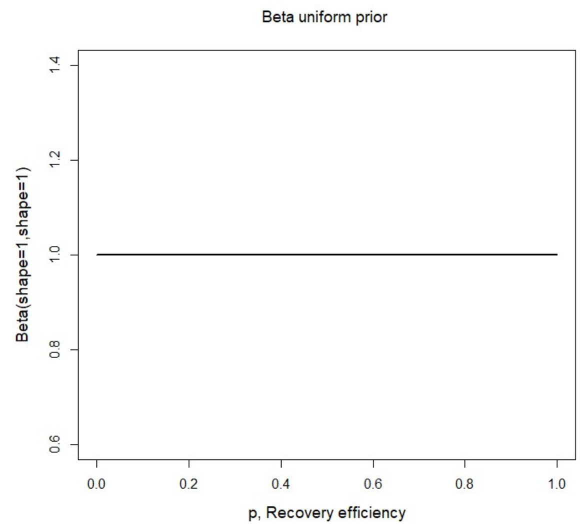



$$x_{ij} \sim Poisson(p_j \cdot \lambda_j \cdot e_{i,j})$$
$$\lambda_j \sim Gamma(\alpha_{prior}; \beta_{prior})$$
$$\alpha_{prior} \sim Gamma(\alpha_0 = 0.5; \beta_0 = 0)$$
$$\beta_{prior} \sim Gamma(\theta_0 = 0.5; \mu_0 = 0)$$
$$p_j \sim Beta(\alpha_p = 1; \beta_p = 1)$$

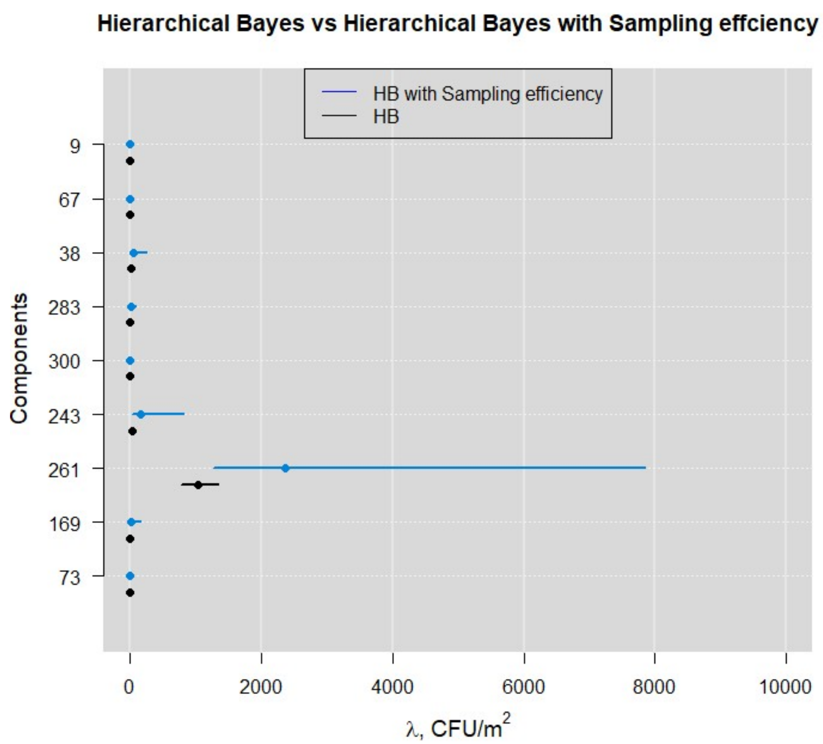
# Recovery Efficiency and Hierarchical Bayes



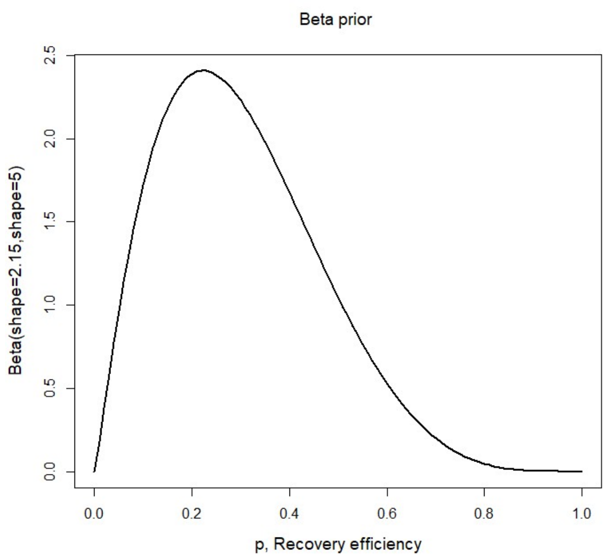

$$x_{ij} \sim Poisson(p_j \cdot \lambda_j \cdot e_{i,j})$$
$$\lambda_j \sim Gamma(\alpha_{prior}; \beta_{prior})$$
$$\alpha_{prior} \sim Gamma(\alpha_0 = 0.5; \beta_0 = 0)$$
$$\beta_{prior} \sim Gamma(\theta_0 = 0.5; \mu_0 = 0)$$
$$p_j \sim Beta(\alpha_p = 1; \beta_p = 1)$$



# Recovery Efficiency and Hierarchical Bayes




$$x_{ij} \sim Poisson(p_j \cdot \lambda_j \cdot e_{i,j})$$
$$\lambda_j \sim Gamma(\alpha_{prior}; \beta_{prior})$$
$$\alpha_{prior} \sim Gamma(\alpha_0 = 0.5; \beta_0 = 0)$$
$$\beta_{prior} \sim Gamma(\theta_0 = 0.5; \mu_0 = 0)$$
$$p_j \sim Beta(\alpha_p = 2.15; \beta_p = 5)$$





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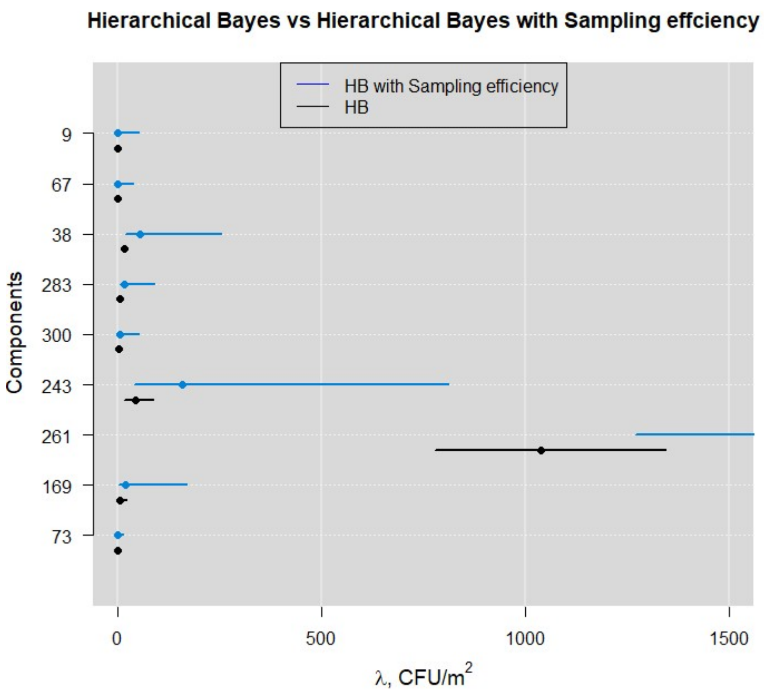
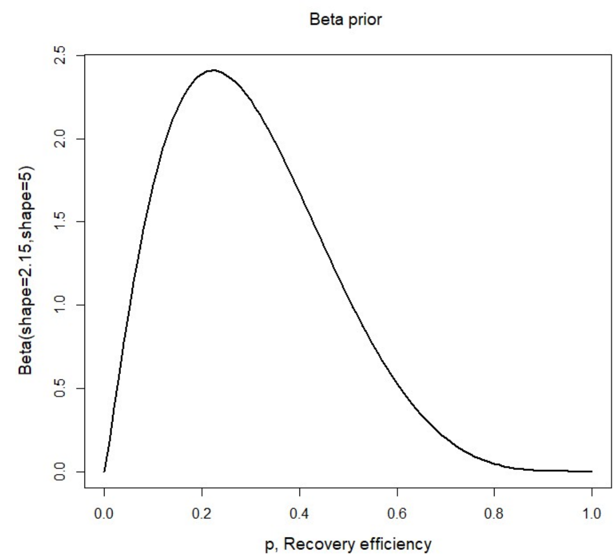
# Recovery Efficiency and Hierarchical Bayes




$$x_{ij} \sim Poisson(p_j \cdot \lambda_j \cdot e_{i,j})$$
$$\lambda_j \sim Gamma(\alpha_{prior}; \beta_{prior})$$
$$\alpha_{prior} \sim Gamma(\alpha_0 = 0.5; \beta_0 = 0)$$
$$\beta_{prior} \sim Gamma(\theta_0 = 0.5; \mu_0 = 0)$$
$$p_j \sim Beta(\alpha_p = 2.15; \beta_p = 5)$$





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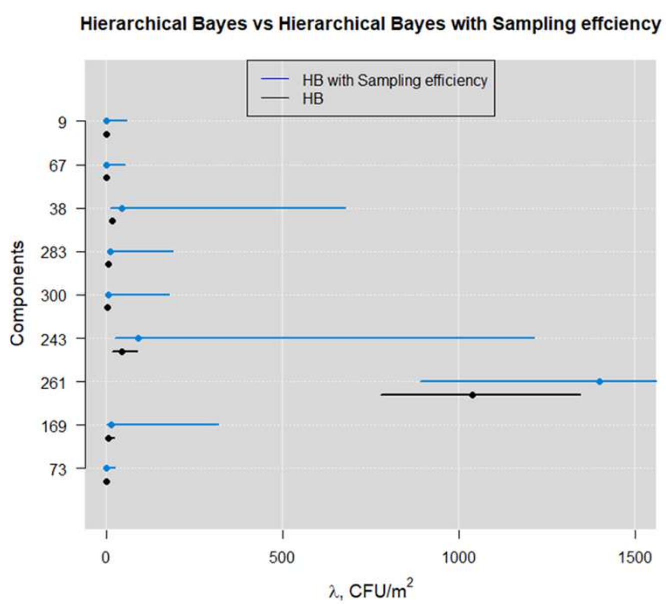
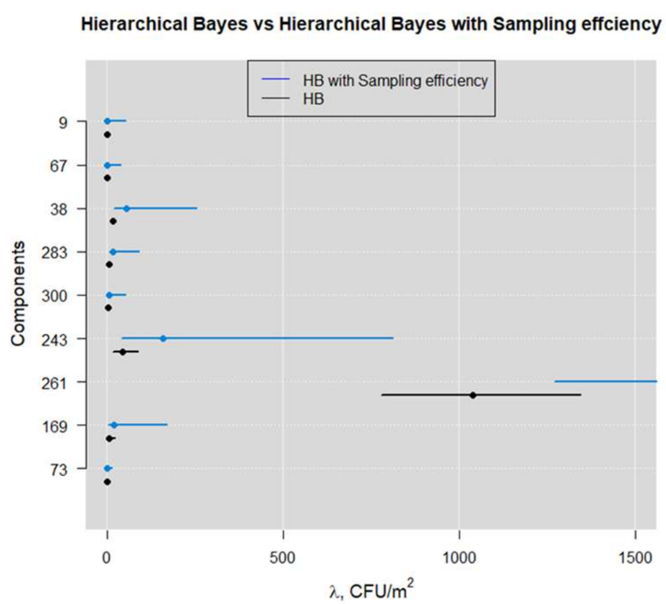
# Recovery Efficiency and Hierarchical Bayes

$p_j \sim Beta(\alpha_p = 1; \beta_p = 1)$




$p_j \sim Beta(\alpha_p = 2.15; \beta_p = 5)$



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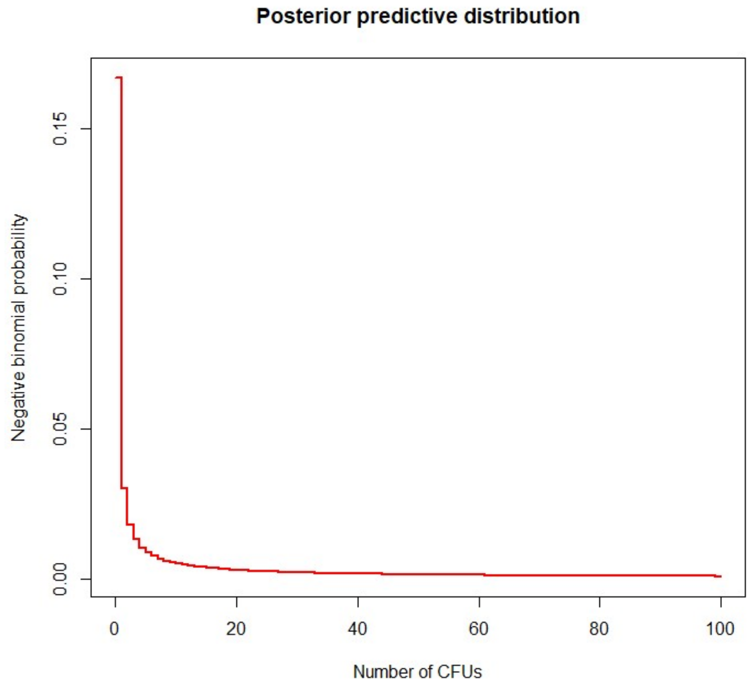
# Posterior Predictive Distribution for all Nine Components




| Component | CFU Count | Area Sampled, $m^2$ | Exposure: Area Sampled*Pour Fraction, $m^2$ | Total Surface of the Component, $m^2$ | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|
| 9 | 0 | 0.6031 | 0.2167 | 0.7580 | 79.5650 |
| 67 | 0 | 0.8575 | 0.2460 | 7.1500 | 11.9930 |
| 38 | 12 | 3.1050 | 0.8065 | 10.0000 | 31.0500 |
| 283 | 5 | 4.5710 | 1.1427 | 12.0000 | 38.0920 |
| 300 | 1 | 2.6600 | 0.6705 | 5.0000 | 53.2000 |
| 243 | 5 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |
| 261 | 52 | 0.0600 | 0.0480 | 0.3120 | 19.2310 |
| 169 | 1 | 0.2400 | 0.1920 | 0.5850 | 41.0260 |
| 73 | 0 | 2.4200 | 0.6160 | 2.7400 | 88.3212 |

$$mean = 3587.032, \frac{CFUs}{m^2}\ ; std = 8.431 \cdot 10^3\ \frac{CFUs}{m^2}; Total\ surface\ area = 38.843, m^2$$

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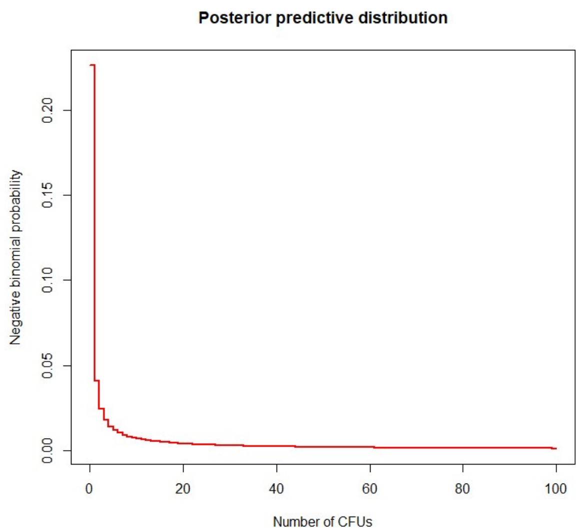
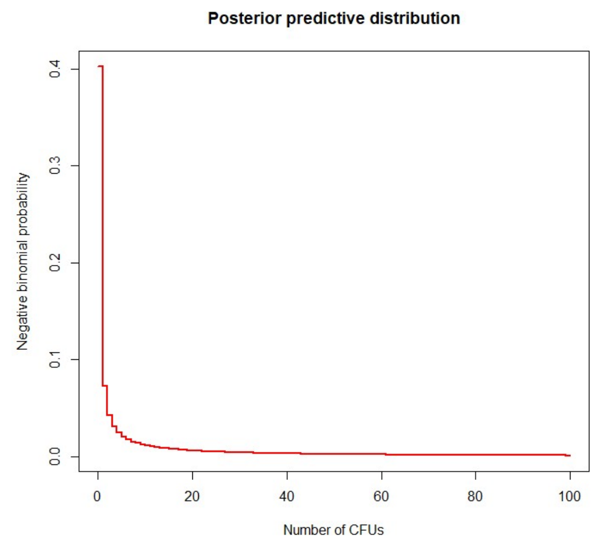
# Posterior Predictive Distribution for Components 67 and 243




$mean = 660, \frac{CFUs}{m^2}\ ; std = 1551\ \frac{CFUs}{m^2}; Total\ surface\ area = 7.1500, m^2$

$mean = 27, \frac{CFUs}{m^2}\ ; std = 64\ \frac{CFUs}{m^2}; Total\ surface\ area = 0.2980, m^2$

| Component | CFU Count | Area Sampled, $m^2$ | Exposure: Area Sampled*Pour Fraction, $m^2$ | Total Surface of the Component, $m^2$ | % Sampled=Area Sampled/Total Area |
|---|---|---|---|---|---|
| 67 | 0 | 0.8575 | 0.2460 | 7.1500 | 11.9930 |
| 243 | 5 | 0.2800 | 0.1140 | 0.2980 | 93.9600 |

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# Back Ups

# Poolability of Data Subsets

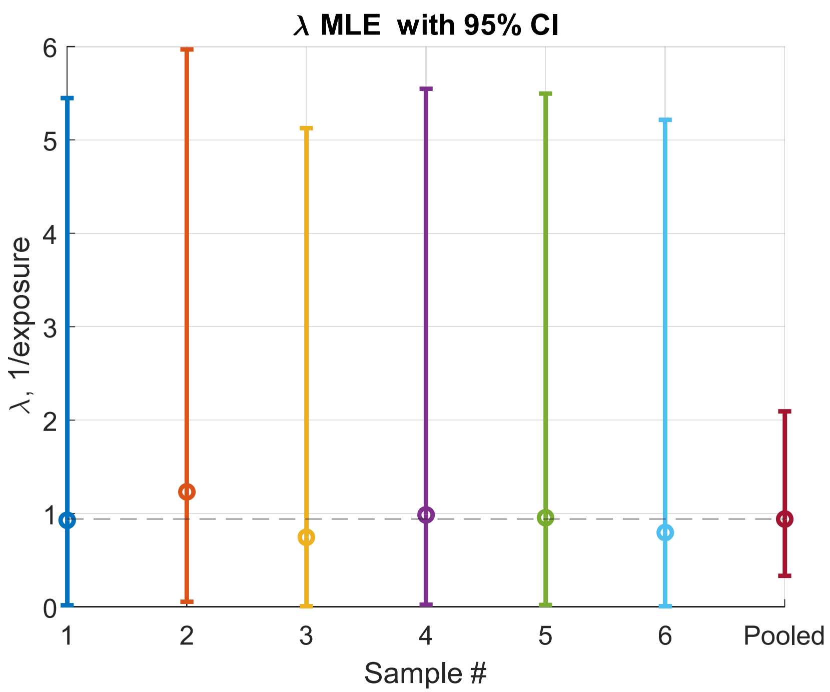
Graphical and Statistical Techniques

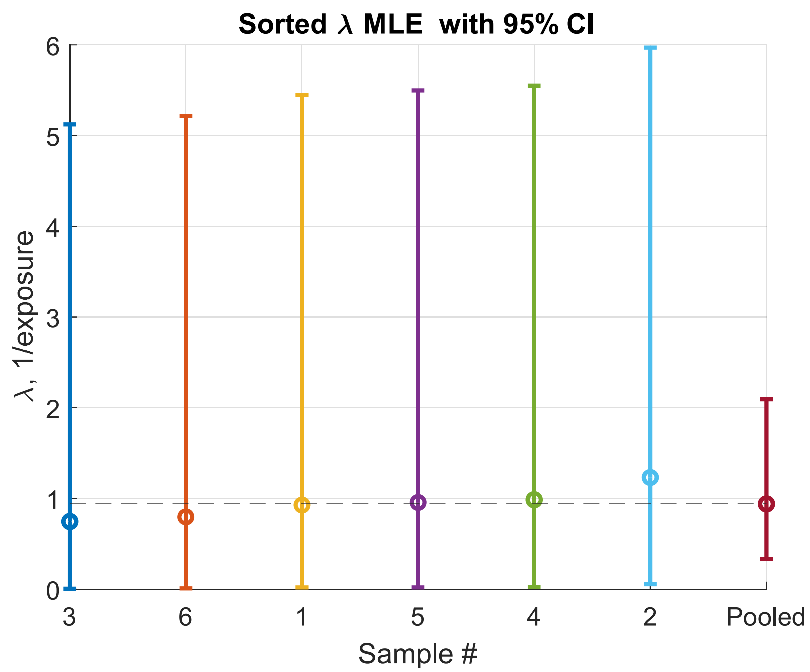
# Check if λ is the same for six plants

| Plant | 1 | 2 | 3 | 4 | 5 | 6 | Pooled |
|---|---|---|---|---|---|---|---|
| Observed count | 4 | 5 | 3 | 5 | 4 | 4 | 26 |
| Exposure, reactor years | 4.31 | 4.06 | 4.02 | 5.07 | 5.23 | 5.02 | 27.71 |
| Expected count | 4.05 | 3.82 | 3.78 | 4.77 | 4.92 | 4.72 | 26.07 |

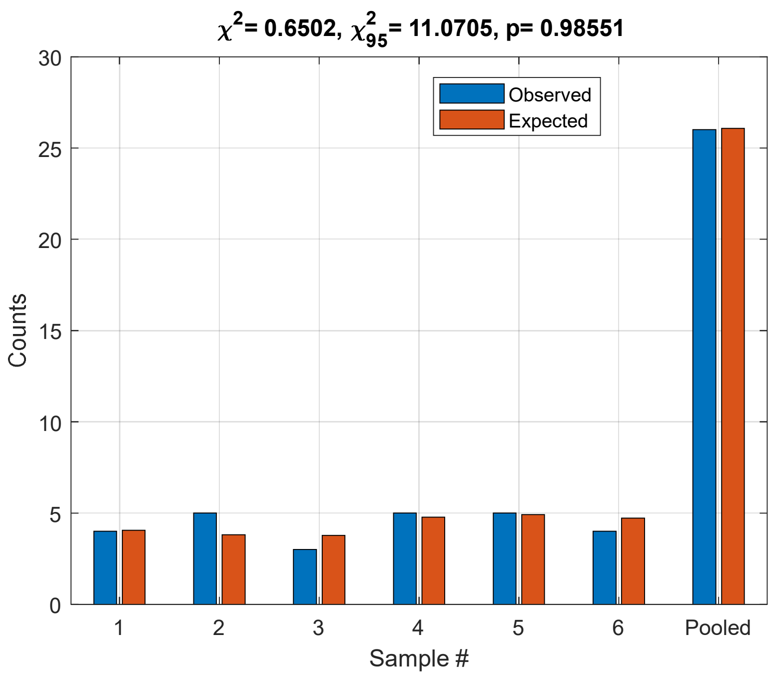
$\lambda_{pooled} = \frac{\sum Observed\ count}{\sum Exposure} = \frac{26}{27.71} = 0.94$, Expected count=$\lambda_{pooled} \cdot Exposure$

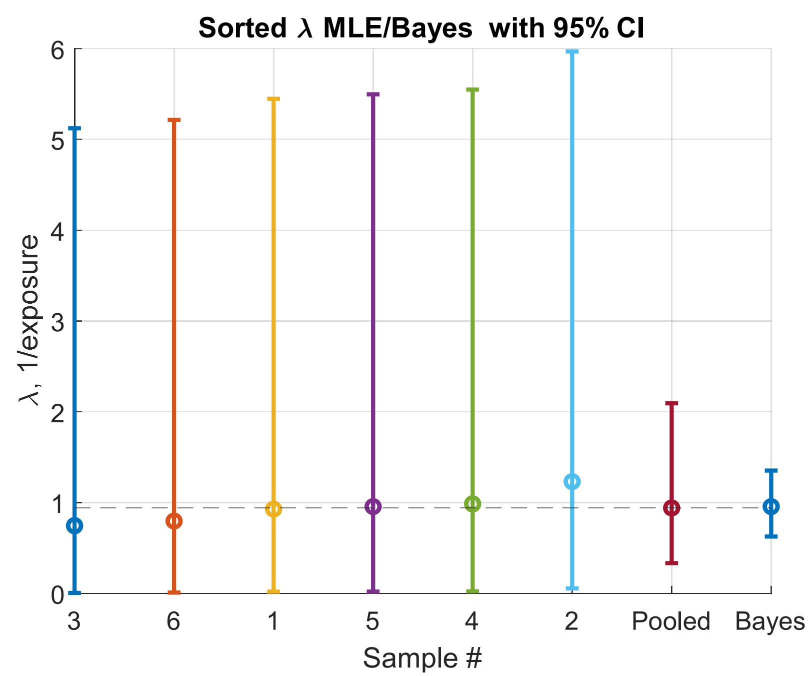
# Graphical Technique for Maximum Likelihood Estimation (MLE)



# Chi-square Test



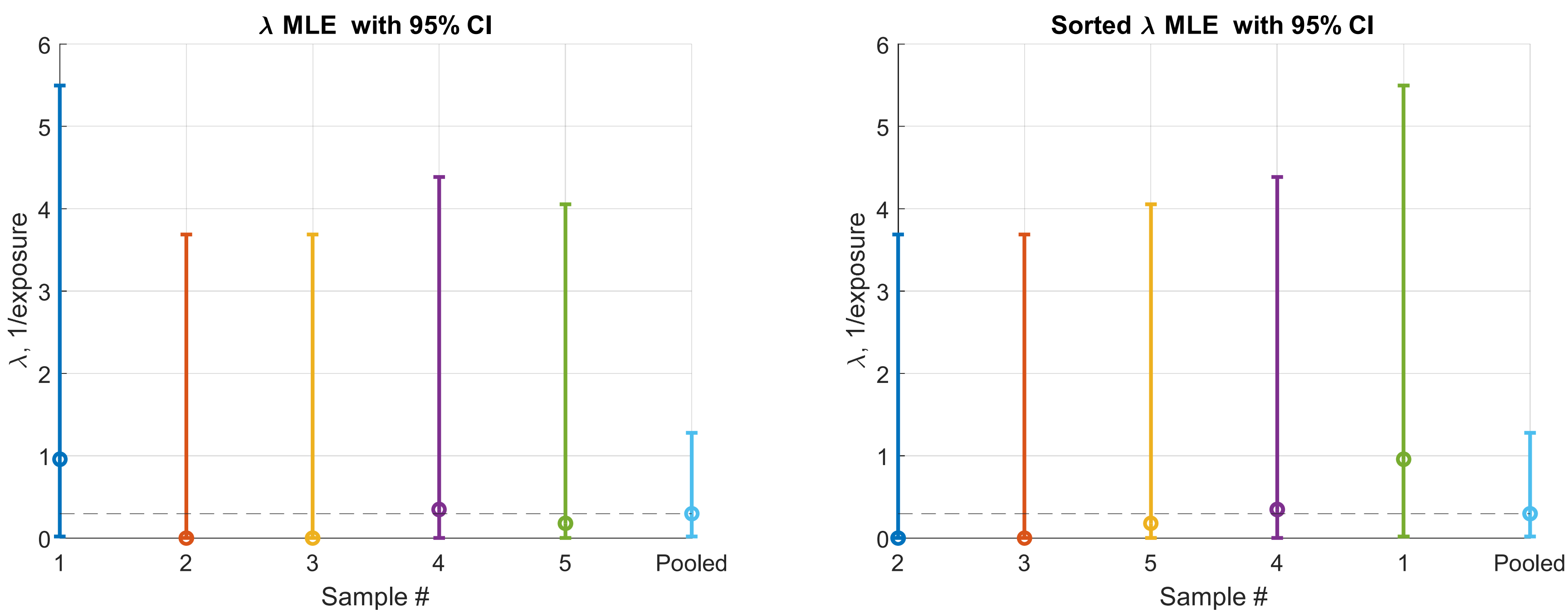




Applicability of chi-square - $\frac{\sum number\ of\ observed\ counts}{number\ of\ samples} \geq 2$

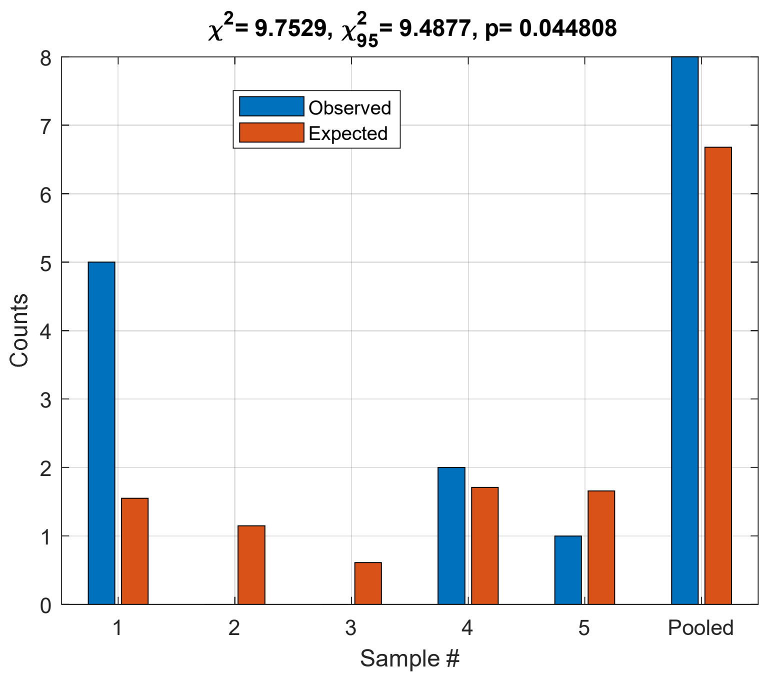
# Borderline Case

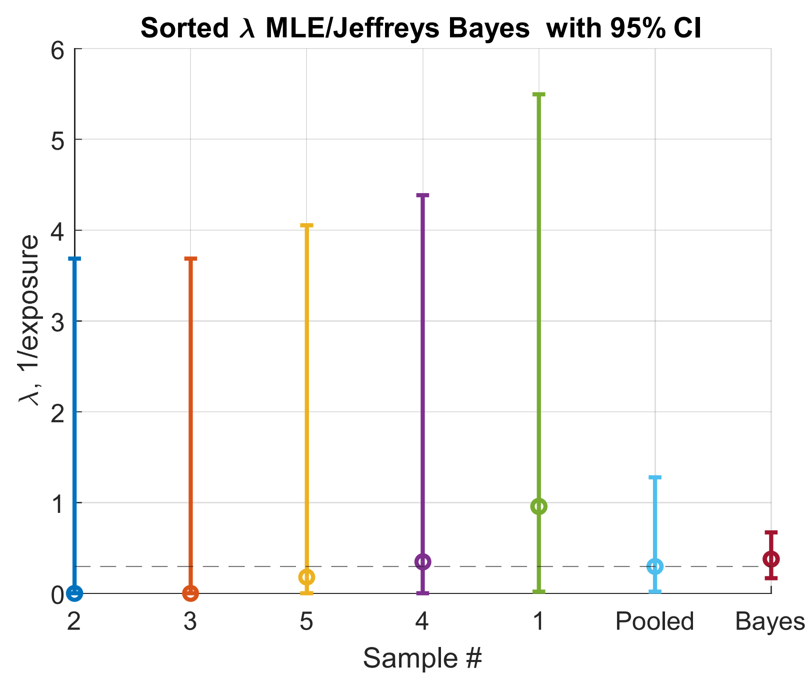
| Plant | 1 | 2 | 3 | 4 | 5 | Pooled |
|---|---|---|---|---|---|---|
| Observed count | 5 | 0 | 0 | 2 | 1 | 8 |
| Exposure, years | 5.224 | 3.871 | 2.064 | 5.763 | 5.586 | 22.508 |
| Expected count | 1.55 | 1.15 | 0.61 | 1.71 | 1.66 | 6.67 |

# Graphical Technique



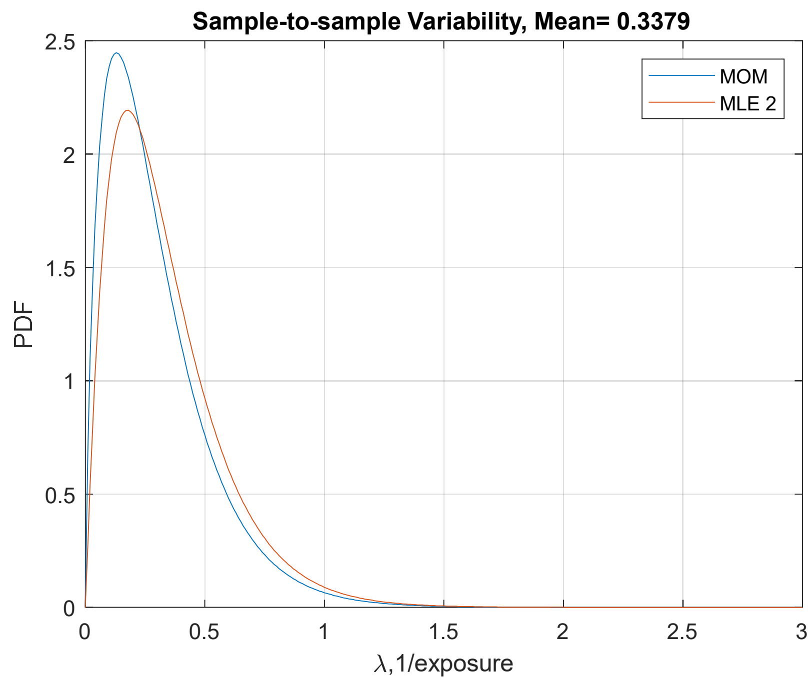
# Chi-square Test



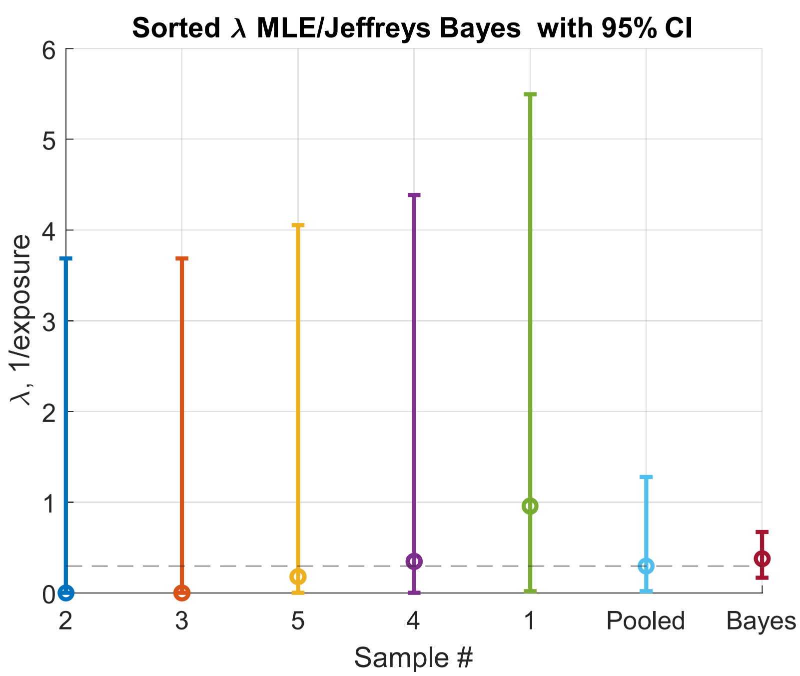



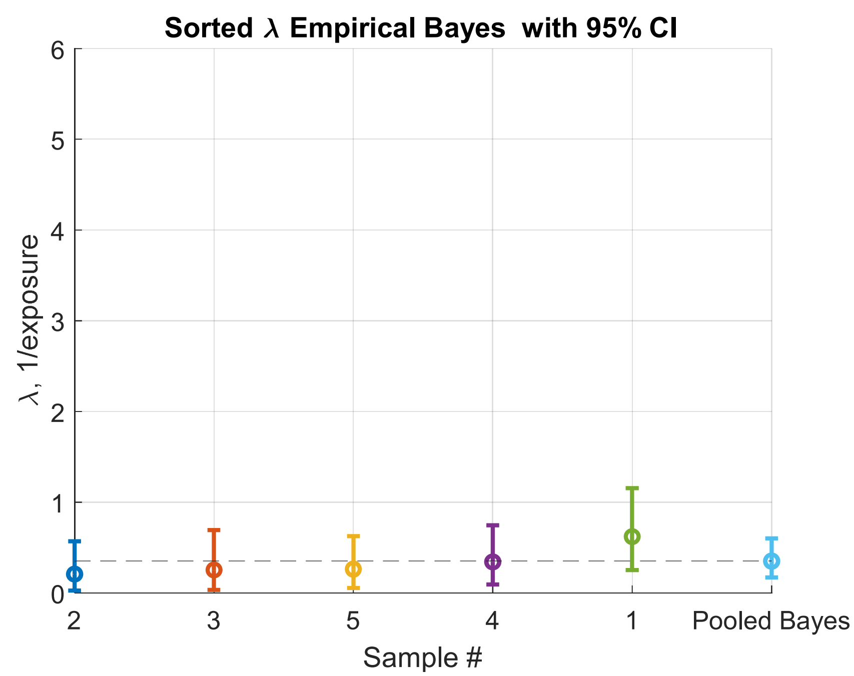

We reject $H_0$ at the 5% significance level, but not at the 2.5% significance level since $\chi^2_{97.5}$ = 11.14. The p-value is between 0.05 and 0.025.

# Sample-to-Sample Variability via Empirical Bayes (EB)

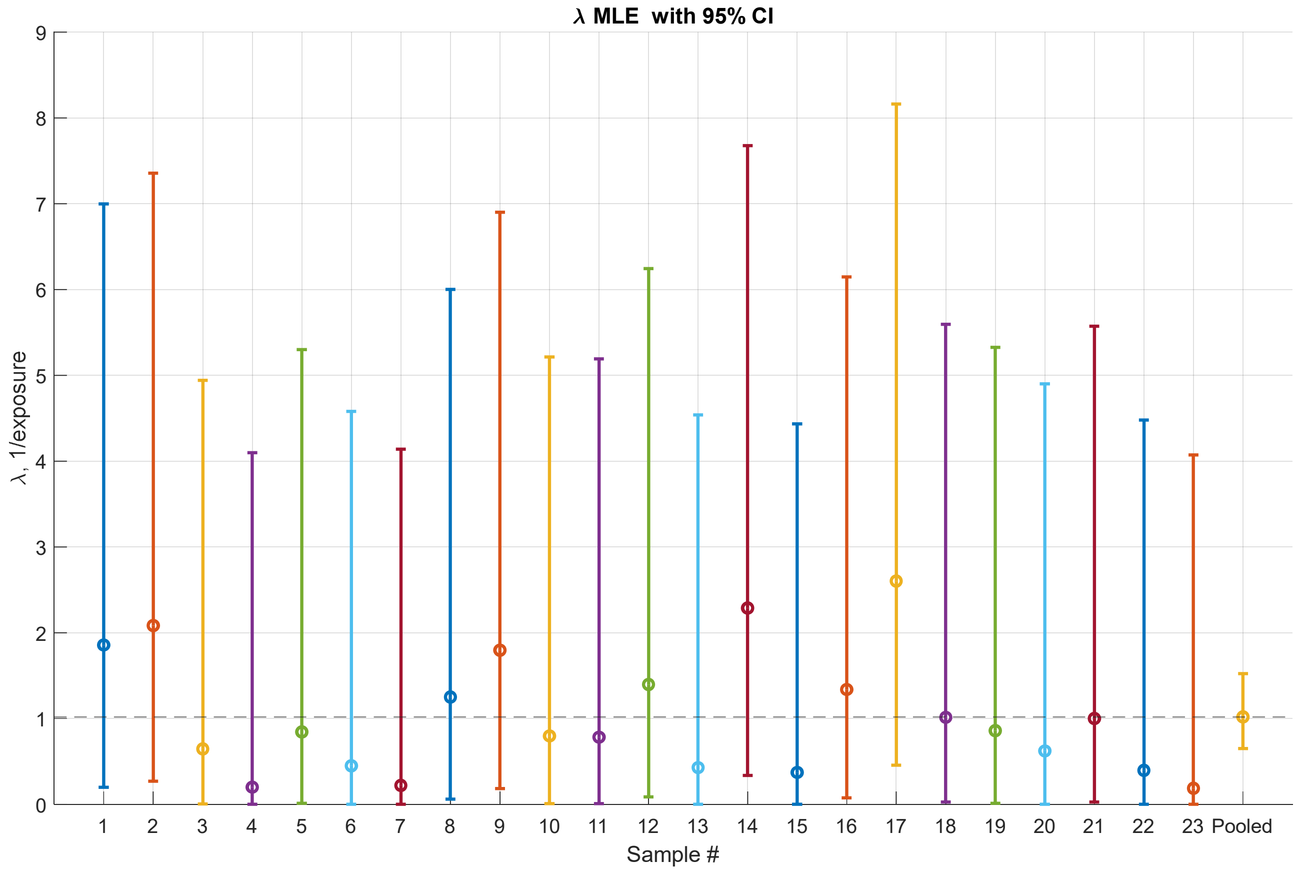


# Empirical Bayes Estimate

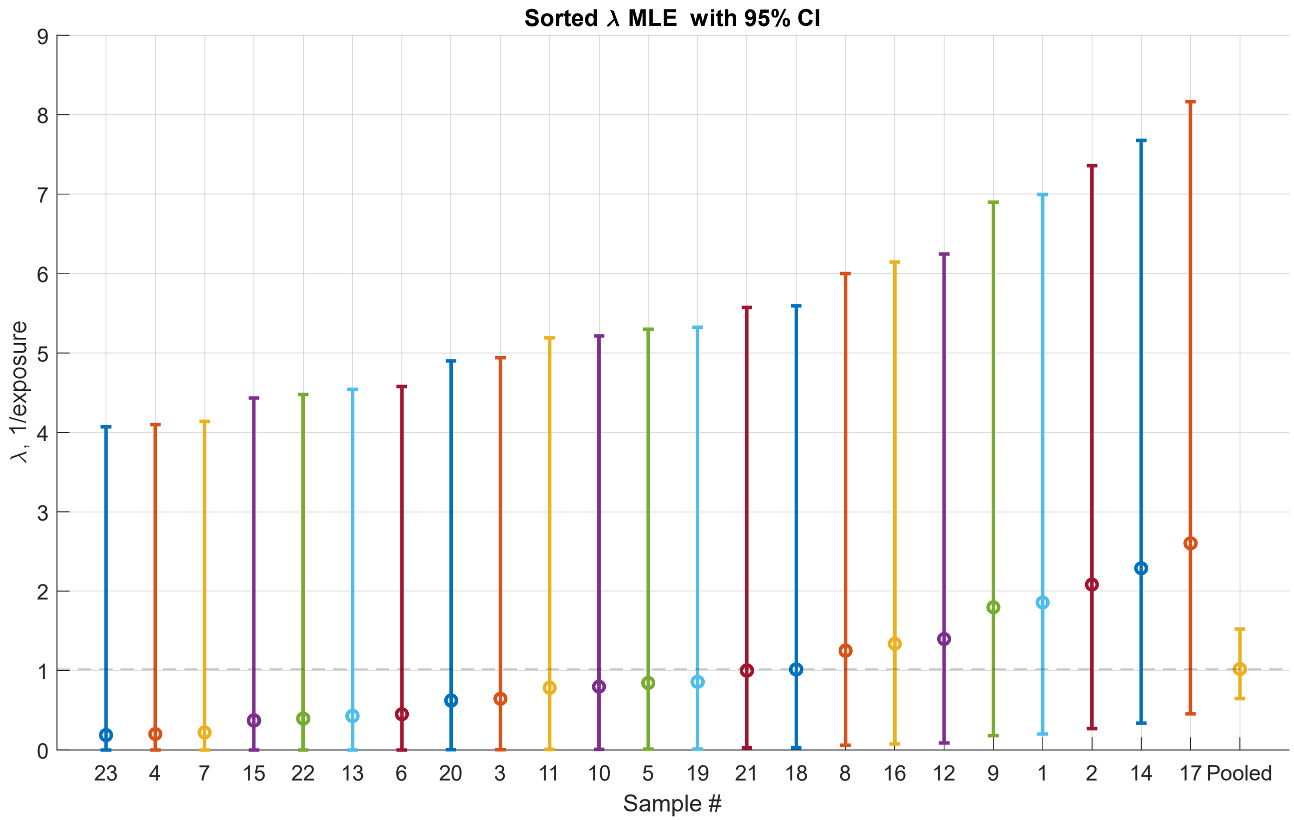


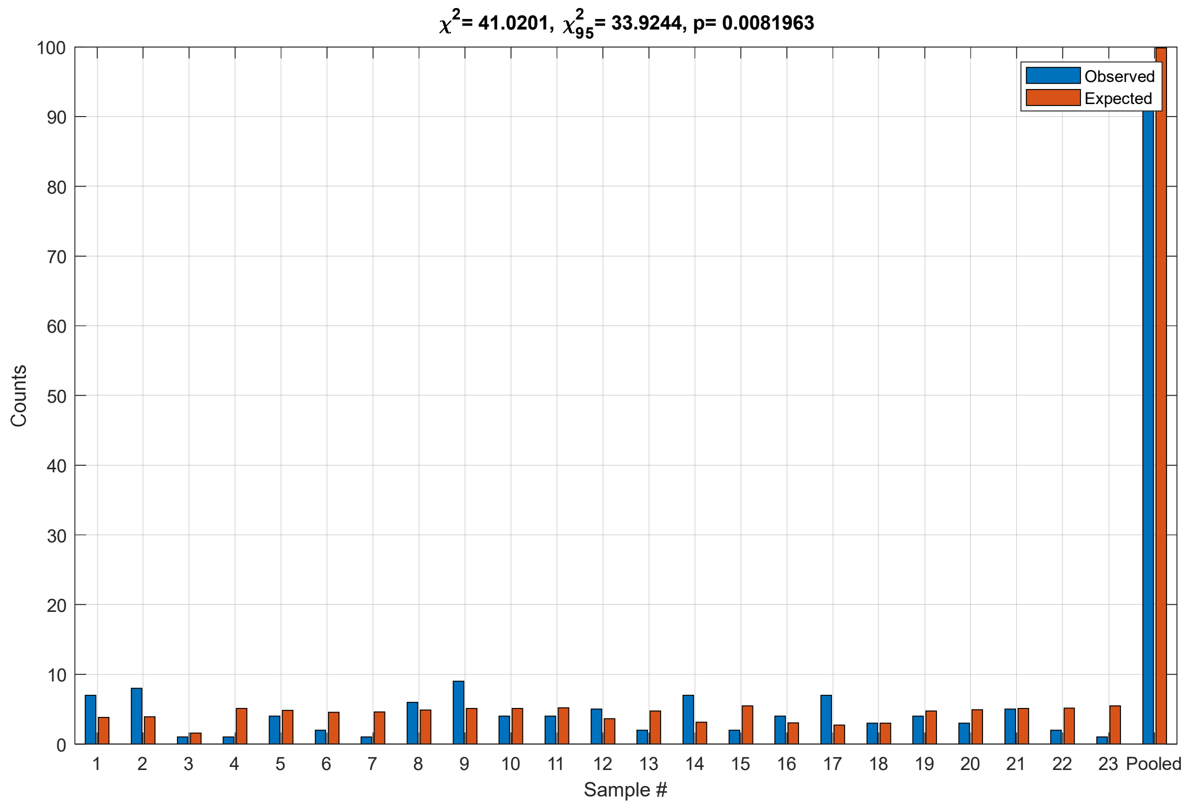
# Non-Poolable Data Set



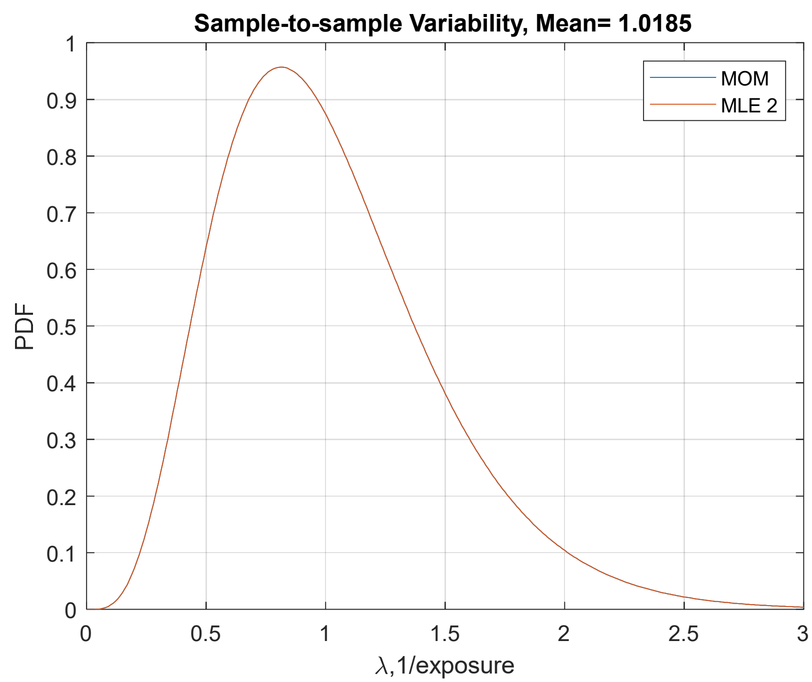
# Non-Poolable Data Set, sorted



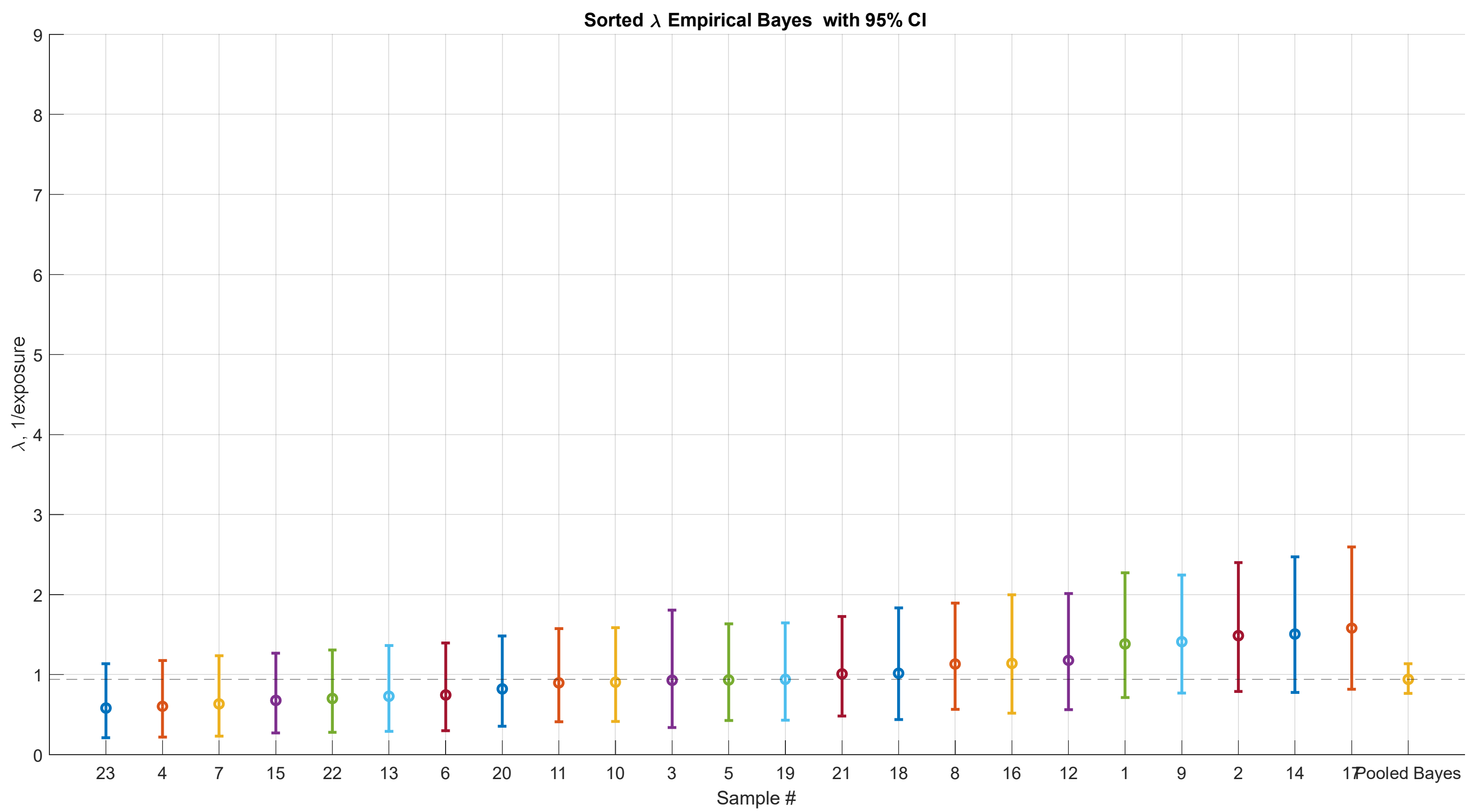
# Chi-square Test



# Sample-to-sample variability via EB



# Empirical Bayes Estimate

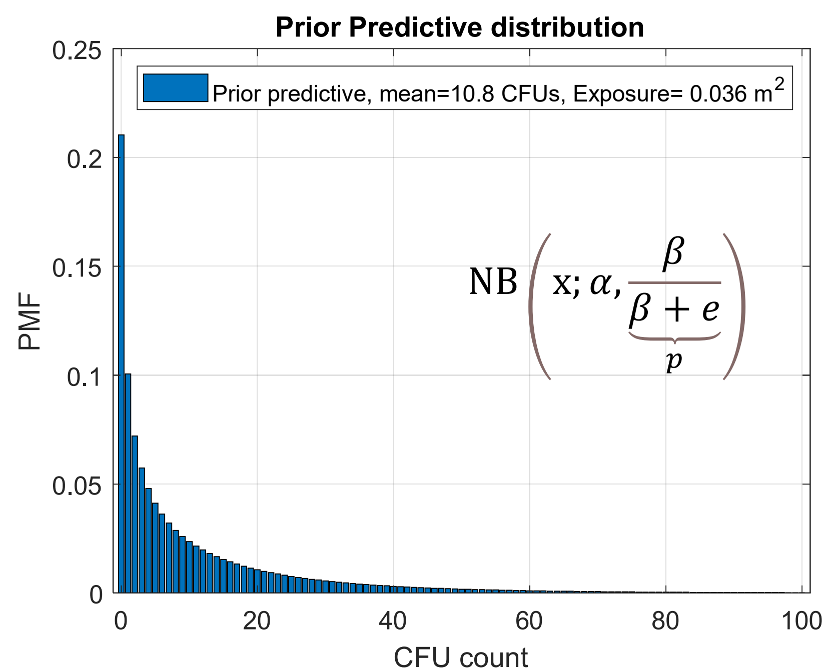


# Component 261

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 1 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 3 | **0.8** | 4 | Component 261 |
| PEB Mating Surface, To PAE | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PEB Mating Surfaces, To PAE | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PEB Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, To PEB | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, to PEB | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 6 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 8 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 14 | **0.8** | 4 | Component 261 |

# Preposterior analysis-Prior predictive distribution with constrained noninformative (CNI) prior: Gamma [α=0.5 β=1/(2·300)] and Poisson likelihood

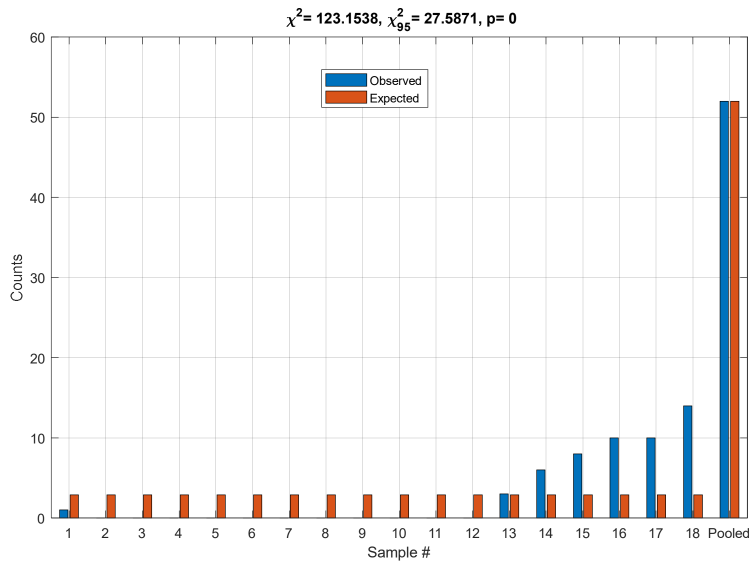
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 1 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 3 | 0.8 | 4 | Component 261 |
| PEB Mating Surface, To PAE | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| PEB Mating Surfaces, To PAE | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| PEB Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| PAE Mating Surface, To PEB | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| PAE Mating Surface, to PEB | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| PAE Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 6 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 8 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | 0.8 | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 14 | 0.8 | 4 | Component 261 |

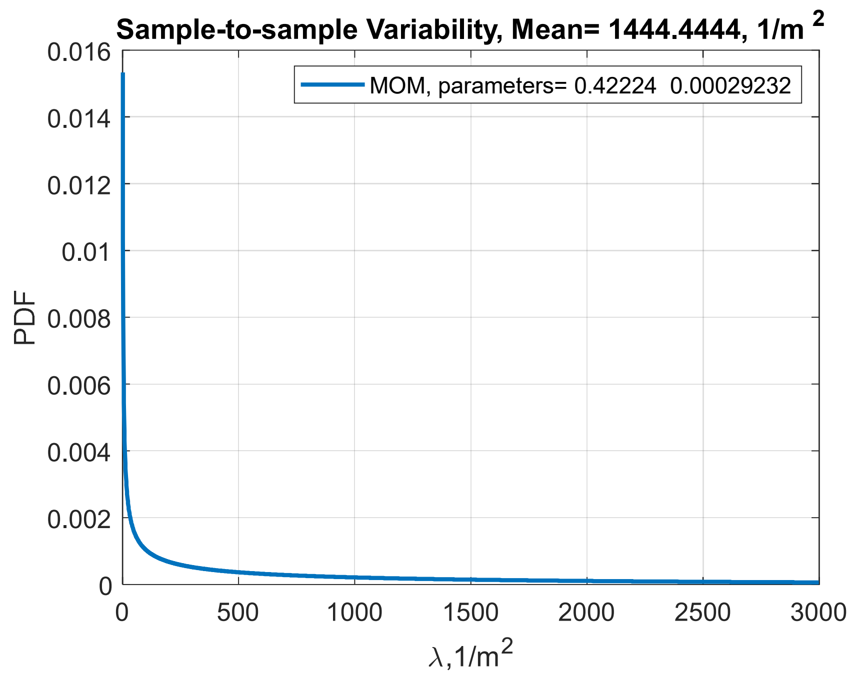



$$90\%\ credible\ interval\ [0 \div 42]\ counts$$

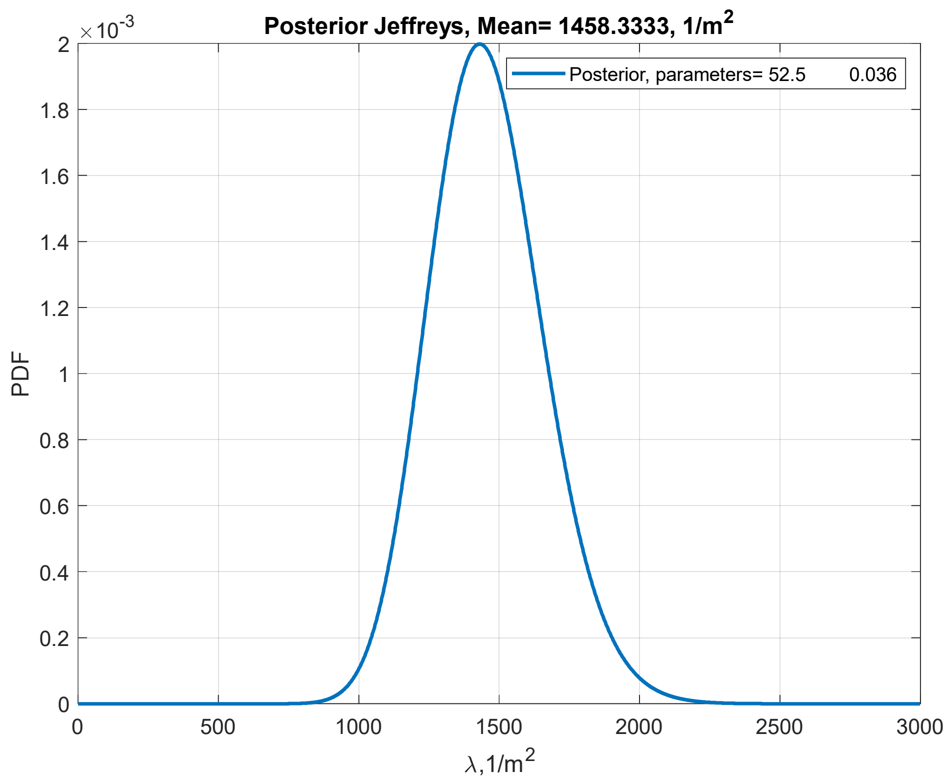
$$P(CFUs \geq 52 = 0.03)$$

# Data Collected on 5/20/2014



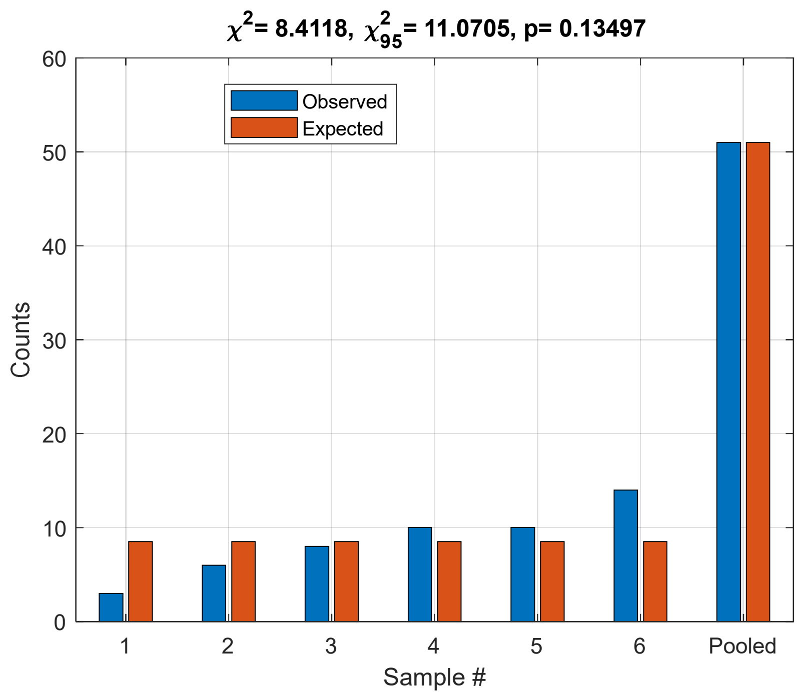



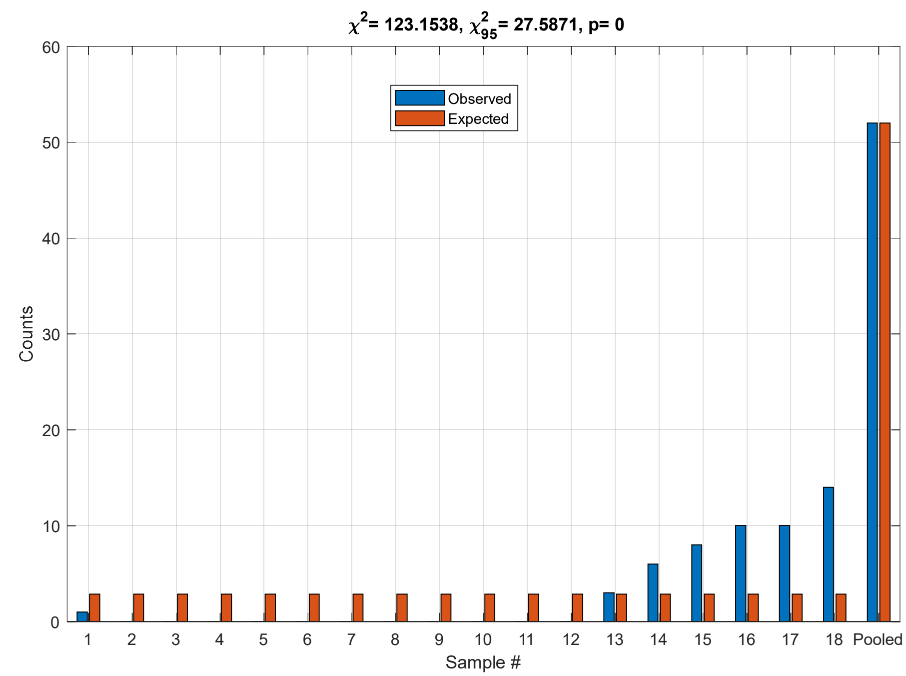
# Pooled 5/20/2014 data with Jeffreys prior



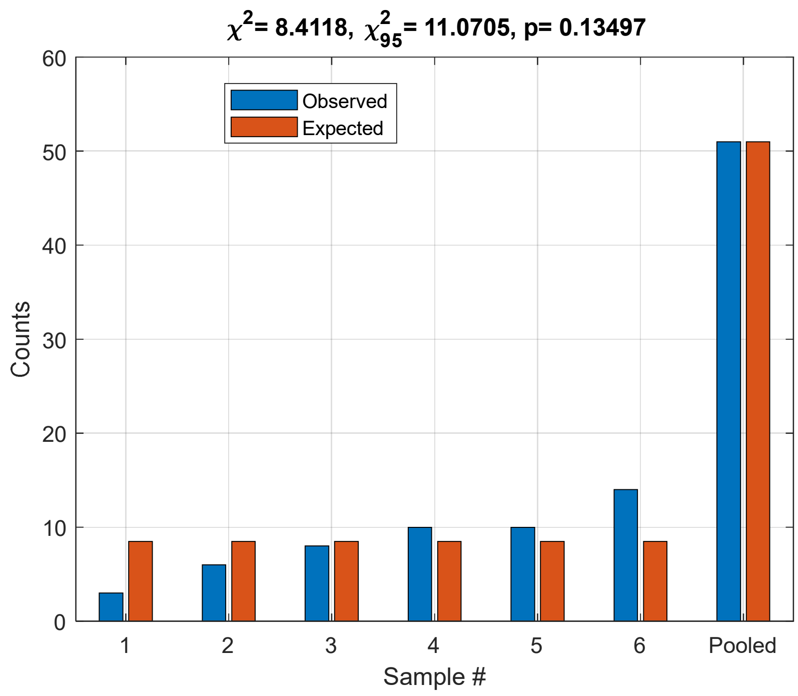

$\lambda$ 90% $credible\ interval$ $[1143.8\ \div 1804.4]\ 1/m^2$

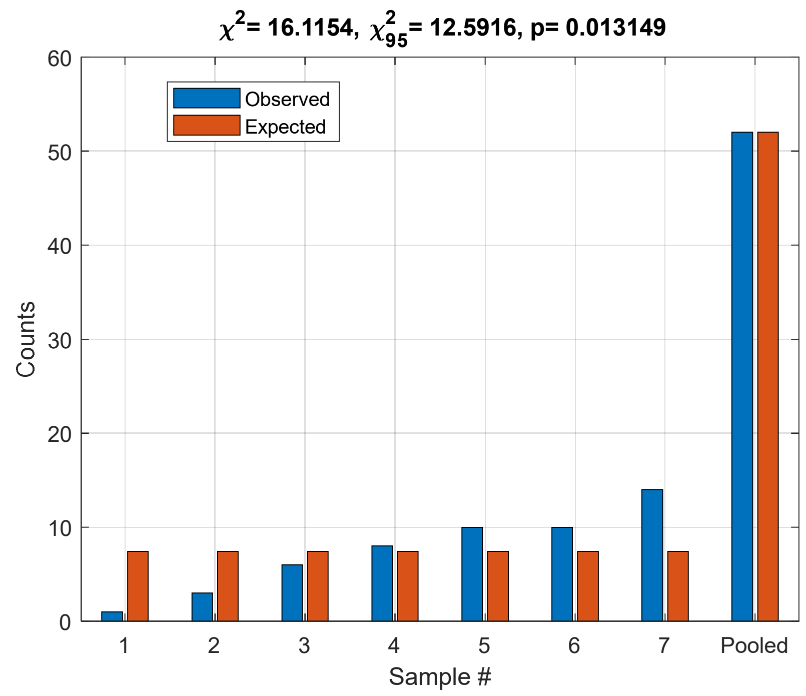
# Poolability test for 5/20/2014 data with zero and 1 counts excluded



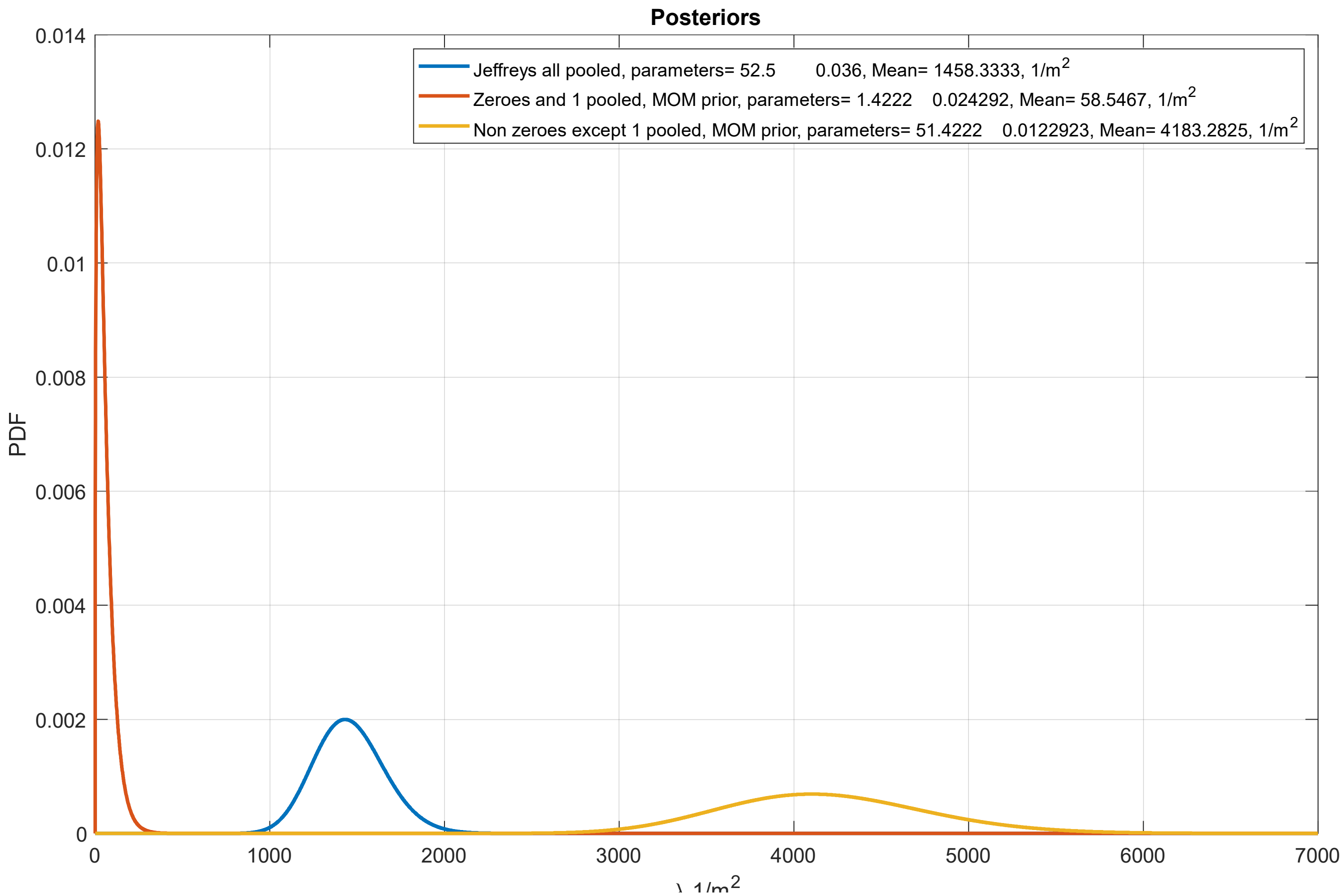



# Poolability test for all nonzero 5/20/2014 data (count of 1 is included)



# Posterior analysis for different pooling scenarios



# Handbook of Parameter Estimation for Probabilistic Risk Assessment. NUREG/CR-6823

- "In actual data analysis, do not stop with the decision that a difference is, or is not, statistically significant. Do not even stop after reporting the p-value. That may be acceptable if the p-value is very small (much less than 0.05) or very large (much larger than 0.05). In many cases, however, statistical significance is far from the whole story. Engineering significance is just as important."
- "Are there engineering reasons for expecting one plant to have a different event rate than the other plants do, either because of the hardware or because of procedures during shutdown? (Be warned that it is easy to find justifications in hindsight, after seeing the data. It might be wise to hide the data and ask these questions of a different knowledge-able person.)"
- "What are the consequences for the PRA analysis if the data are pooled or if, instead, one plant is treated separately from the other plants? **Does the decision to pool or not make any practical difference?** "

# Poolability-Partial Poolabilty-NonPoolability

- For poolable data each sample has the same sampled/population mean
- How to pool nonpoollable data?
- Why to pool/partially pool nonpoolable data?
- Partial poolability-compromise between population mean and individual samples
- How partially poolability models are treating zero CFUs?
- Performance of partially pooled models
- Integration of partially pooled models with spore density analysis model
- Aggregation of partially poolable models
- Hierarchical Bayes
- Summary statistics for reporting
- Patrial poolability for ALL sampled data

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 1 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 3 | **0.8** | 4 | Component 261 |
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| PEB Mating Surfaces, To PAE | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PEB Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, To PEB | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, to PEB | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| PAE Mating Surface, Mated Surface to | 0.0025 | 7/10/2017 | swab | 0 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 6 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 8 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 10 | **0.8** | 4 | Component 261 |
| P/N 10360619-1 Rev B S/N 101 | 0.0025 | 5/20/2014 | Swab | 14 | **0.8** | 4 | Component 261 |

# Gamma-Poisson Model, single sample

$$P(\lambda/x) = \frac{\underbrace{\frac{(\lambda\cdot e)^x}{x!}e^{-\lambda\cdot e}}_{Likelihood}.\underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}}.\lambda^{\alpha_{prior}-1}.e^{-\lambda\cdot\beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior}}{\int_0^\infty \underbrace{\frac{(\lambda\cdot e)^x}{x!}e^{-\lambda\cdot e}}_{Likelihood}.\underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}}.\lambda^{\alpha_{prior}-1}.e^{-\lambda\cdot\beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior}d\lambda} = Gamma(\underbrace{x+\alpha_{prior}}_{\alpha_{post}}, \overbrace{e+\beta_{prior}}^{\beta_{post}})$$

$$E_{prior}(\lambda/\alpha_{prior},\beta_{prior}) = \frac{\alpha_{prior}}{\beta_{prior}}$$

$$\lambda = \frac{x}{e}\ ; Maximum\ Likelihood\ Estimation\ (MLE)$$

$$E_{post}(\lambda/x,\alpha_{prior},\beta_{prior}) = \frac{\underbrace{x+\alpha_{prior}}_{\alpha_{post}}}{\overbrace{e+\beta_{prior}}^{\beta_{post}}}$$

*x-CFU counts*

*λ- bioburden density, CFUs/m²*

*e- exposure, pour ratio*area sampled, m²*

*α, β-parameters of prior distribution*

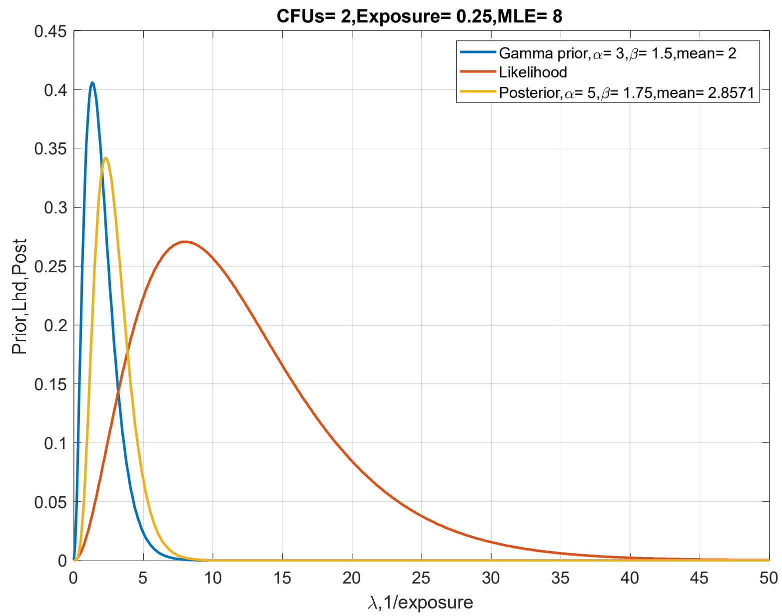
We want to estimate bioburden density λ from a single CFU observation-x, e in the Bayesian situation

# Gamma-Poisson Model

$$P(\lambda/x) = \frac{\underbrace{\frac{(\lambda \cdot e)^x}{x!} e^{-\lambda \cdot e}}_{Likelihood} . \underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}} . \lambda^{\alpha_{prior}-1} . e^{-\lambda \cdot \beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior}}{\int_0^\infty \underbrace{\frac{(\lambda \cdot e)^x}{x!} e^{-\lambda \cdot e}}_{Likelihood} . \underbrace{\frac{\beta_{prior}{}^{\alpha_{prior}} . \lambda^{\alpha_{prior}-1} . e^{-\lambda \cdot \beta_{prior}}}{\Gamma(\alpha_{prior})}}_{Prior} d\lambda} = Gamma(\underbrace{x + \alpha_{prior}}_{\alpha_{post}}, \overbrace{e + \beta_{prior}}^{\beta_{post}})$$

$$E_{prior}(\lambda/\alpha_{prior}, \beta_{prior}) = \frac{\alpha_{prior}}{\beta_{prior}}$$

$$E_{post}(\lambda/x, \alpha_{prior}, \beta_{prior}) = \frac{\underbrace{x + \alpha_{prior}}_{\alpha_{post}}}{\overbrace{e + \beta_{prior}}^{\beta_{post}}}$$



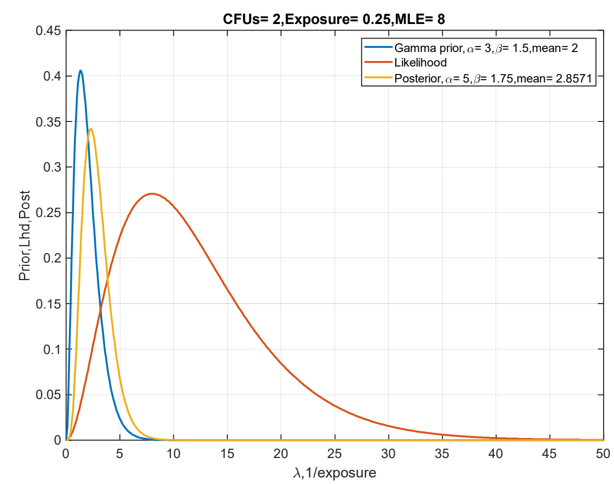
# Different Types of Prior

$$E_{post}\left(\lambda/x, \alpha_{prior}, \beta_{prior}\right) = \frac{\overbrace{x + \alpha_{prior}}^{}\,\alpha_{post}}{\beta_{post}\,\underbrace{\mathrm{e} + \beta_{prior}}_{}}$$

$$E(\lambda|x) = \frac{x + \alpha_{prior}}{\mathrm{e} + \beta_{prior}} = \left[\frac{e}{\mathrm{e} + \beta_{prior}}\right] \cdot \left(\frac{x}{e}\right) + \left[\frac{\beta_{prior}}{\mathrm{e} + \beta_{prior}}\right] \cdot \left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = [1 - B] \cdot \left(\frac{x}{e}\right) + [B] \cdot \left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$= \left(\frac{x}{e}\right) - [B] \cdot \left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta}{\mathrm{e} + \beta_{prior}}\right] \cdot \left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{\mathrm{e} + \beta_{prior}} \leq 1$$



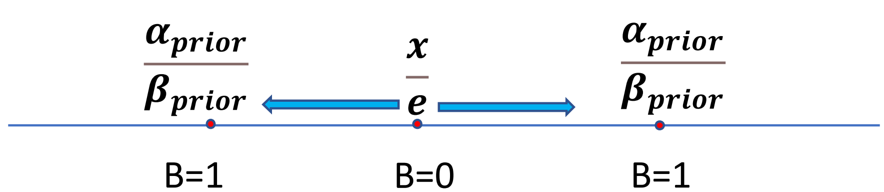
# Shrinkage as Pooling

$$E(\lambda|x) = \frac{x+\alpha_{prior}}{\mathrm{e}+\beta_{prior}} = \left[\frac{e}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e}\right) + \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$= \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\lambda)}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}} \le 1 \qquad \lim_{\beta_{prior}\to 0}\frac{\beta_{prior}}{e+\beta_{prior}} = 0 \qquad \lim_{\beta_{prior}\to\infty}\frac{\beta_{prior}}{e+\beta_{prior}} = 1 \qquad E(\lambda) = \frac{\alpha}{\beta}, Var(\lambda) = \frac{\alpha}{\beta^2}$$

$$\lim_{e\to 0}\frac{\beta_{prior}}{e+\beta_{prior}} = 1 \qquad \lim_{e\to\infty}\frac{\beta_{prior}}{e+\beta_{prior}} = 0$$



# Recap

$$E(\lambda|x) = \frac{x+\alpha_{prior}}{\mathrm{e}+\beta_{prior}} = \left[\frac{e}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e}\right) + \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

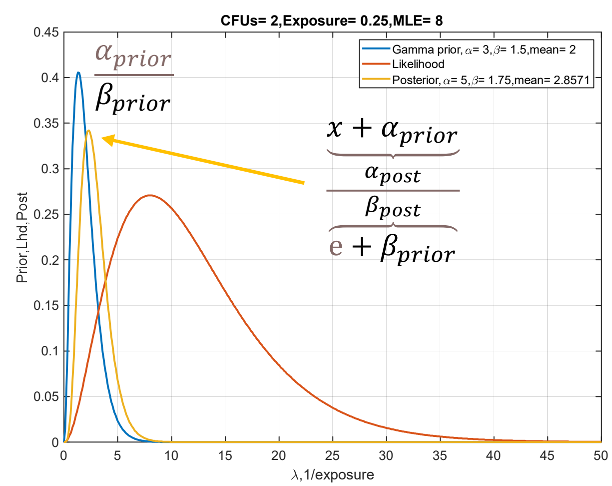
$$= \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}(\lambda)}}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}} \leq 1$$

$$\mathrm{Mode}(\lambda|x) = \frac{x+\alpha_{prior}-1}{\mathrm{e}+\beta_{prior}}, \textit{Maximum a posteriori (MAP) estimate}$$

Talking Points

1. Bayesian estimate (posterior mean value) is a compromise between data and prior
2. The compromise (degree of shrinkage) is controlled by shrinkage (regularization) parameter – B
3. Bayesian estimate is shrunken (pulled) toward prior mean
4. Parameter B is a function of exposure (amount of evidence) and prior's precision (beta parameter)
5. As we sample more surface, the data are weighted more heavily
6. Variance of posterior



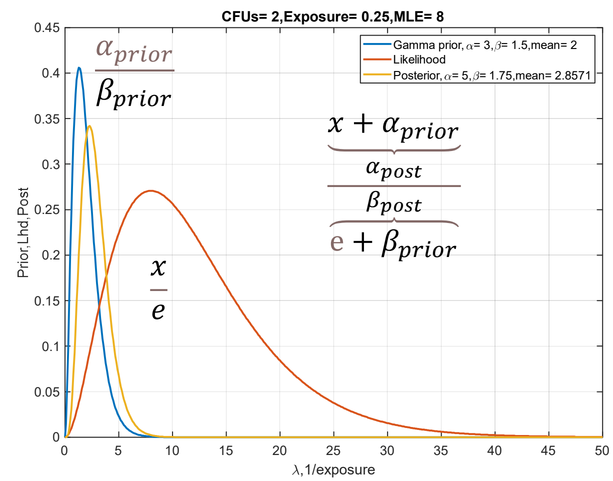
# Uncertainty Estimation for Posterior Inference

$$\lambda = \frac{x}{e}, Var(\lambda) = \frac{x}{e} = 8$$

$$E_{prior}(\lambda) = \frac{\alpha_{prior}}{\beta_{prior}}, Var(\lambda) = \frac{\alpha_{prior}}{\beta_{prior}{}^2} = 1.33$$

$$E_{post}(\lambda|x) = \frac{x + \alpha_{prior}}{\mathrm{e} + \beta_{prior}}, Var(\lambda|x) = \frac{x + \alpha_{prior}}{(\mathrm{e} + \beta_{prior})^2} = 1.63$$

$$\mathrm{Mode}(\lambda|x) = \frac{x+\alpha_{prior}-1}{\mathrm{e}+\beta_{prior}} = \frac{2+3-1}{0.25+1.5} = \frac{4}{1.75} = 2.2857$$

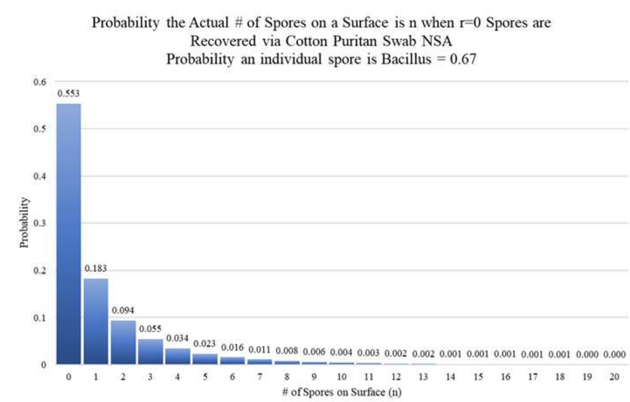


# Treatment of zeros by different priors

| Prior | α,β | E(λ\|x) | E(λ\|X=0) |
|---|---|---|---|
| Jeffreys | Gamma(0.5,0) | $\frac{x+\alpha}{e+\beta} = \frac{x}{e} + \frac{0.5}{e}$ | $\frac{0.5}{e}$ |
| Uniform | Gamma(1,0) | $\frac{x+\alpha}{e+\beta} = \frac{x}{e} + \frac{1}{e}$ | $\frac{1}{e}$ |
| Max Entropy | Gamma(1,1/μ) | $\frac{\mu(x+1)}{e \cdot \mu + 1}$ | $\frac{\mu}{e \cdot \mu + 1}$ |
| Constrained noninformative (CNI) | Gamma(0.5, 1/(2·μ)) | $\frac{2 \cdot \mu(x+0.5)}{2 \cdot e \cdot \mu + 1}$ | $\frac{\mu}{2 \cdot e \cdot \mu + 1}$ |
| Gamma prior | Gamma(α, β) | $\frac{x+\alpha}{e+\beta}$ | $\frac{\alpha}{e+\beta}$ |
| | | | |

$$E_{post}(\lambda / x, \alpha_{prior}, \beta_{prior}) = \frac{\overbrace{x + \alpha_{prior}}^{\alpha_{post}}}{\underbrace{e + \beta_{prior}}_{\beta_{post}}}$$

$$\text{Gamma}(\lambda; \alpha, \beta) = \frac{\beta^{\alpha} \cdot \lambda^{\alpha-1} \cdot e^{-\lambda \cdot \beta}}{\Gamma(\alpha)}$$



# Poolable and Nonpoolable Data Sets

| Item Name | Sample Device | Area Sampled, $m^2$ | Pour Fraction | Exposure,$m^2$ | CFUs | Component Association |
|---|---|---|---|---|---|---|
| Cruise Stage - Outer Cylinder Section | wipe | 0.75 | 0.25 | 0.1875 | 1 | Component 300 |
| CS +Y Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| CS -Y Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| CS +X Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| Cruise Stage - Inner Cylinder Section | wipe | 0.75 | 0.25 | 0.1875 | 0 | Component 300 |
| Cruise Stage - Cruise Stage - Inner Cylindrical Section, metal surfaces between electronic boxes | wipe | 0.75 | 0.25 | 0.1875 | 0 | Component 300 |
| CS bottom mount ring | wipe | 0.3 | 0.25 | 0.075 | 0 | Component 300 |
| Inside CS primary structure | wipe | 0.1 | 0.25 | 0.025 | 0 | Component 300 |
| Lander - Inside MLI Radar Electronics | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |

# Loss/Risk/Error Functions-Quantifying Quality of a Parameter Estimate

$P(X = x|\lambda_{true}) = \frac{(\lambda_{true} \cdot e)^x}{x!} e^{-\lambda_{true} \cdot e}, x = 0,1,2, \ldots, \lambda_{true} \in (0, \infty)$, e$\in (0, \infty)$

*x-CFU counts*

*λ- bioburden density, CFUs/m²*

*e- exposure, pour ratio*area sampled, m²*

$E[X] = \lambda_{true} \cdot e, Var[X] = \lambda_{true} \cdot e$

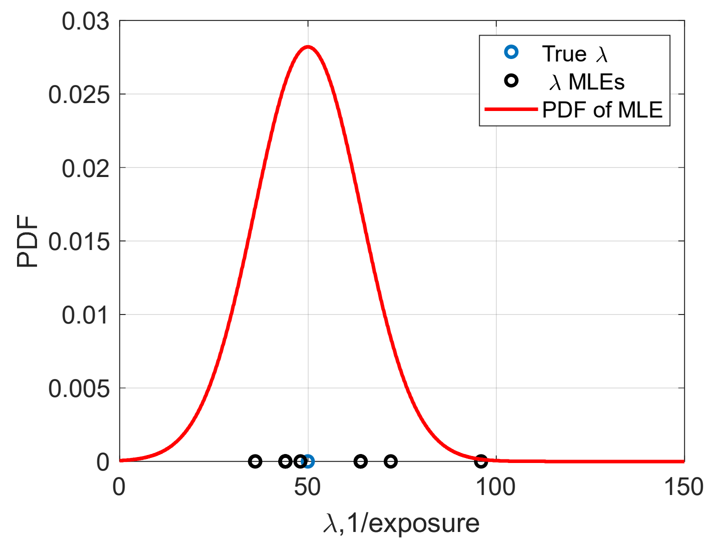
$\hat{\lambda}_{MLE} = \frac{x}{e}$ ; *Maximum Likelihood Estimation (MLE)* $\qquad \hat{\lambda}_{MLE} = \frac{x + \epsilon}{e}$

$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e} E[x] = \frac{1}{e} \cdot (\lambda_{true} \cdot e) = \lambda_{true}$

$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2} Var[x] = \frac{1}{e^2} \cdot (\lambda_{true} \cdot e) = \frac{\lambda_{true}}{e}$

$Loss = \left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right]$, *Squared difference*

$Risk = MSE = E\left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right]$, *Mean Squared Error (MSE)*



# Loss/Risk/Error Functions-Quantifying Quality of a Parameter Estimate (multiple measurements)

$P\left(X_i = x_i \middle| \lambda_{true}^i\right) = \frac{(\lambda_{true}^i)^{x_i}}{x_i!} e^{-\lambda_{true}^i \cdot e_i}, x = 0,1,2,\dots, \lambda_{true} \in (0,\infty)$, e$\in$ $(0,\infty)$

$$X = (X_1, X_2, \dots X_n) \quad e = (e_1, e_2, \dots e_n) \quad \lambda = (\lambda_1, \lambda_2, \dots \lambda_n)$$

$$Z = \sum_{i=1}^{n} X_i \quad E = \sum_{i=1}^{n} e_i \quad \Lambda = \sum_{i=1}^{n} \lambda_i$$

$$E[X] = \lambda_{true} \cdot e, Var[X] = \lambda_{true} \cdot e$$

$$\hat{\lambda}_{MLE} = \frac{x}{e} \text{; } Maximum\ Likelihood\ Estimation\ (MLE) \qquad \hat{\lambda}_{MLE} = \frac{x+\epsilon}{e}$$

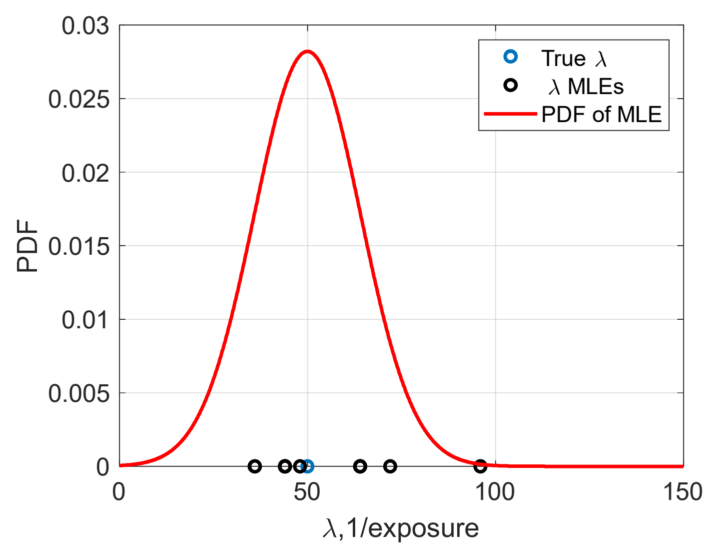
$$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e}E[x] = \frac{1}{e} \cdot (\lambda_{true} \cdot e) = \lambda_{true}$$

$$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2}Var[x] = \frac{1}{e^2} \cdot (\lambda_{true} \cdot e) = \frac{\lambda_{true}}{e}$$

$$Loss = \left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right], Squared\ difference$$

$$Risk = MSE = E\left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right], Mean\ Squared\ Error\ (MSE)$$

*x-CFU counts*
*λ- bioburden density, CFUs/m²*
*e- exposure, pour ratio*area sampled, m²*



# Loss/Risk/Error Functions-Quantifying Quality of a Parameter Estimate (multiple measurements)

$P\left(X_i = x_i \middle| \lambda_{true}^i\right) = \frac{(\lambda_{true}^i)^{x_i}}{x_i!} e^{-\lambda_{true}^i \cdot e_i}, x = 0,1,2, \ldots \lambda_{true}^i \in (0, \infty)$, e$\in (0, \infty)$

$X = (X_1, X_2, \ldots X_n) \quad e = (e_1, e_2, \ldots e_n) \quad \lambda = (\lambda_1, \lambda_2, \ldots \lambda_n)$

$$Z = \sum_{i=1}^{n} X_i \quad E = \sum_{i=1}^{n} e_i \quad \Lambda = \sum_{i=1}^{n} \lambda_i$$

# Bias and Variance of the Estimate/Estimator

$$Bias(\hat{\lambda}) = E[\hat{\lambda}] - \lambda_{true}$$

$$Var(\hat{\lambda}) = E[(\hat{\lambda} - E[\hat{\lambda}])^2] = E[\hat{\lambda}^2] - (E[\hat{\lambda}])^2$$

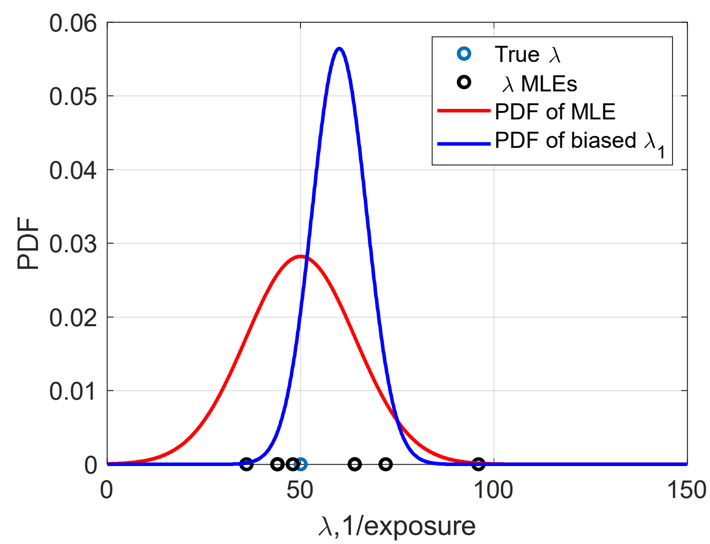
$$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e}E[x] = \frac{1}{e} \cdot (\lambda_{true} \cdot e) = \lambda_{true}$$

$$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2}Var[x] = \frac{1}{e^2} \cdot (\lambda_{true} \cdot e) = \frac{\lambda_{true}}{e}$$

Estimand: parameter to be estimated-$\lambda_{true}$

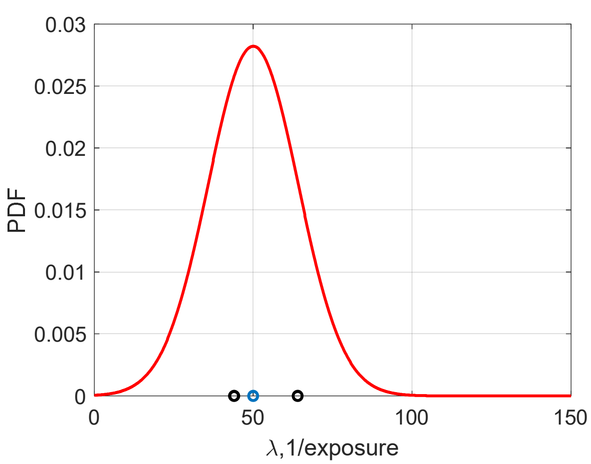
Estimator: the rule (formula) which is used to estimate the parameter of interest-$\hat{\lambda} = \frac{x}{e}$ using the data- x, e

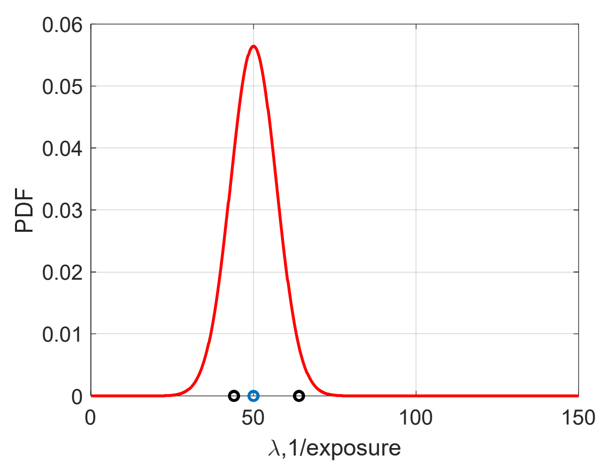
Estimate: the result of applying the estimator to the data , $\hat{\lambda} = 5\ \text{CFUs}/m^2$

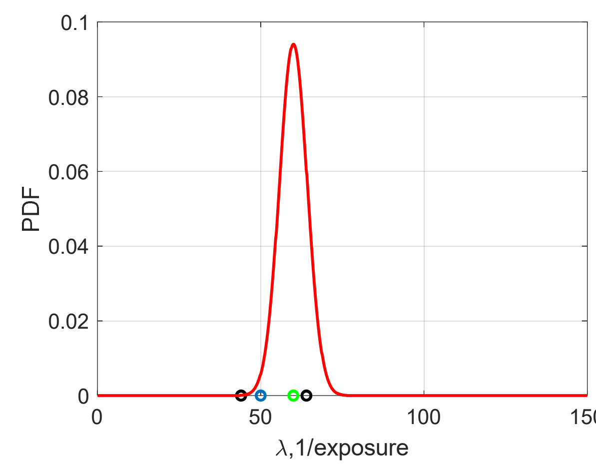


# Mean Squared Error: Bias-Variance Decomposition

$$MSE = E\left[(\hat{\lambda} - \lambda_{true})^2\right] = E\left[(\hat{\lambda} - E[\hat{\lambda}] + E[\hat{\lambda}] - \lambda_{true})^2\right] = E\left[(\hat{\lambda} - E[\hat{\lambda}])^2 + (E[\hat{\lambda}] - \lambda_{true})^2 + 2 \cdot (\hat{\lambda} - E[\hat{\lambda}]) \cdot (E[\hat{\lambda}] - \lambda_{true})\right] = E\left[(\hat{\lambda} - E[\hat{\lambda}])^2\right] + E\left[\,(E[\hat{\lambda}] - \lambda_{true})^2\right] + \underbrace{E\left[2 \cdot (\hat{\lambda} - E[\hat{\lambda}]) \cdot (E[\hat{\lambda}] - \lambda_{true})\right]}_{0} = \underbrace{E\left[(\hat{\lambda} - E[\hat{\lambda}])^2\right]}_{Var(\hat{\lambda})} + \underbrace{(E[\hat{\lambda}] - \lambda_{true})^2}_{Bias(\hat{\lambda})^2}$$



# Bias-Variance Decomposition-Maximum Likelihood Estimator

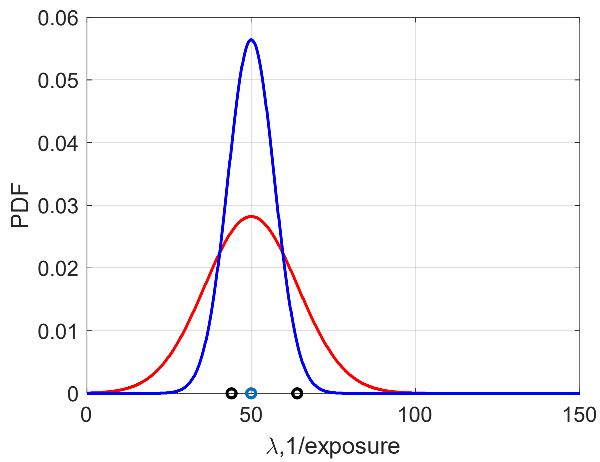
$$\hat{\lambda}_{MLE} = \frac{x}{e}\ ; Maximum\ Likelihood\ Estimation\ (MLE)$$

$$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e}E[x] = \frac{1}{e}\cdot(\lambda_{true}\cdot e) = \lambda_{true}$$

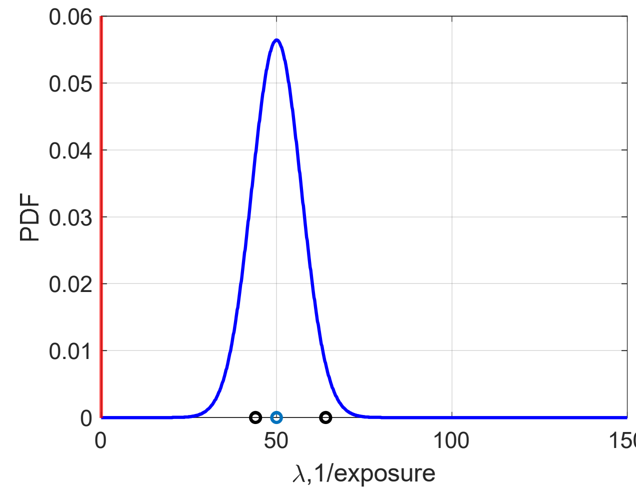
$$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2}Var[x] = \frac{1}{e^2}\cdot(\lambda_{true}\cdot e) = \frac{\lambda_{true}}{e}$$

$$MSE_{MLE} = \underbrace{E\left[(\hat{\lambda}_{MLE} - E[\hat{\lambda}_{MLE}])^2\right]}_{Var(\hat{\lambda})} + \underbrace{(E[\hat{\lambda}_{MLE}] - \lambda_{true})^2}_{Bias(\hat{\lambda})^2=0}$$

$$MSE_{MLE} = \underbrace{E\left[(\hat{\lambda}_{MLE} - E[\hat{\lambda}_{MLE}])^2\right]}_{Var(\hat{\lambda})} = \frac{\lambda_{true}}{e}$$



# Bias-Variance Decomposition- Zero (Constant) Estimator




$$\hat{\lambda}_0 \equiv 0\,; Zero\ estimator\ ignores\ the\ data$$

$$E[\hat{\lambda}_0] = E[0] = 0$$

$$Var[\hat{\lambda}_0] = Var[0] = 0$$

$$MSE_0 = \underbrace{E[(0 - E[0])^2]}_{Var(\hat{\lambda})=0} + \underbrace{(E[0] - \lambda_{true})^2}_{Bias(\hat{\lambda})^2} = {\lambda_{true}}^2$$

$$MSE_{MLE} = \frac{\lambda_{true}}{e}$$

$${\lambda_{true}}^2 < \frac{\lambda_{true}}{e} = \lambda_{true} \cdot \lambda_{true} < \lambda_{true} \cdot \frac{1}{e}; \lambda_{true} < \frac{1}{e}$$

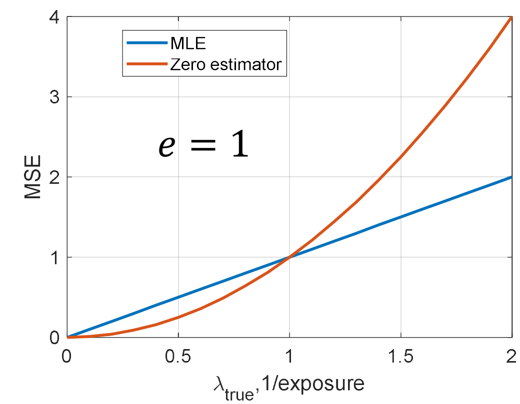
$$\begin{cases} e < 1, \lambda_{true} < \dfrac{1}{e} \\ e = 1, \lambda_{true} < 1 \\ e > 1, \lambda_{true} < \dfrac{1}{e} \end{cases}$$

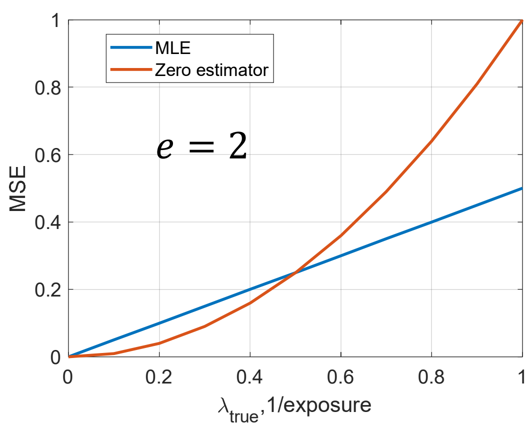
# Bias-Variance Decomposition- Zero (Constant) Estimator – Domination over MLE

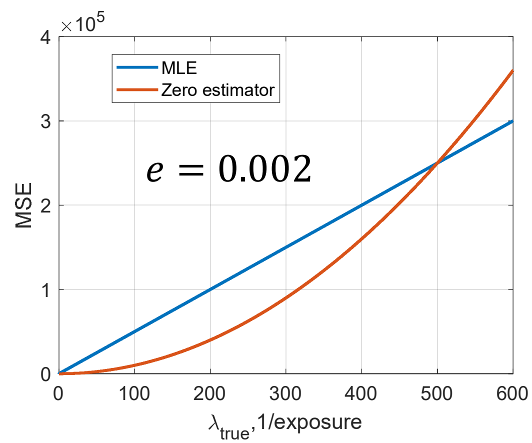
$$MSE_0 = {\lambda_{true}}^2, MSE_{MLE} = \frac{\lambda_{true}}{e}; {\lambda_{true}}^2 < \frac{\lambda_{true}}{e} = \lambda_{true} \cdot \lambda_{true} < \lambda_{true} \cdot \frac{1}{e}; \lambda_{true} < \frac{1}{e}$$

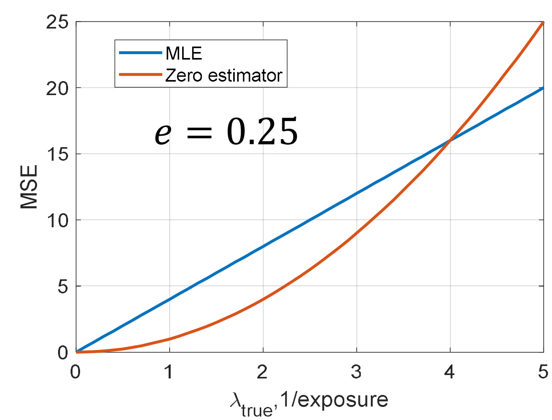
$$MSE_{MLE} = \frac{\lambda_{true}}{e}$$

$$\begin{cases} e < 1, \lambda_{true} < \dfrac{1}{e} \\ e = 1, \lambda_{true} < 1 \\ e > 1, \lambda_{true} < \dfrac{1}{e} \end{cases}$$



# Insight Bioburden Densities

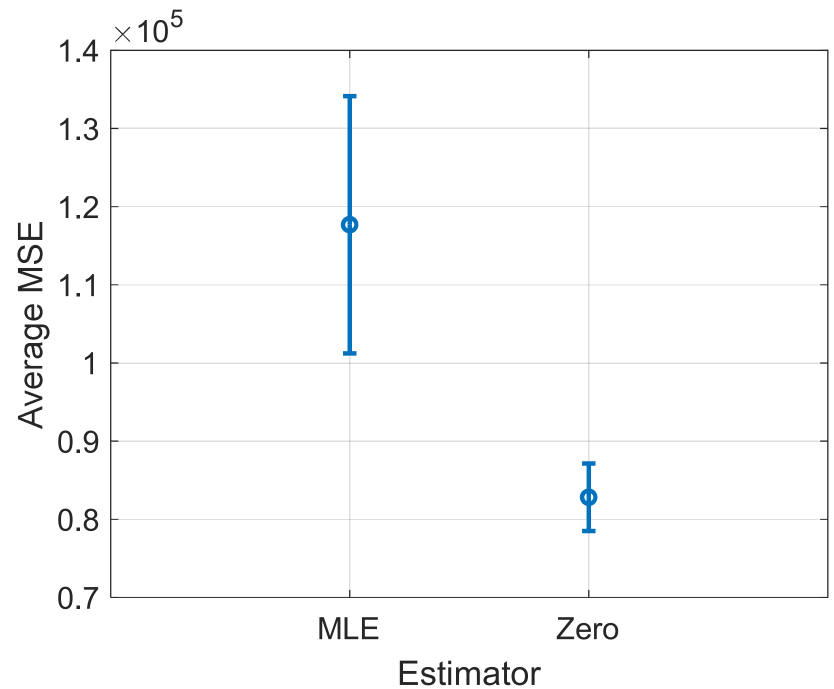
| | Proposed Bayesian Approach (CNI prior) | | | MSL-based 3 sigma (NASA Legacy) | InSight-based weighted average technique (NASA Current) |
|---|---|---|---|---|---|
| Component | Posterior Mean Bioburden Density – λ, CFU/$m^2$ | $5^{th}$ Percentile of Posterior Distribution | $95^{th}$ Percentile of Posterior Distribution | 3 sigma Bioburden Density – λ, CFU/$m^2$ | Weighted Average Bioburden Density – λ, CFU/$m^2$ |
| 9 | 2.2889 | 0.0090 | 8.7928 | 13.84 | 27.99 |
| 73 | 0.8095 | 0.0032 | 3.1097 | 4.87 | 17.36 |
| 300 | 2.2315 | 0.2617 | 5.8130 | 5.96 | 9.54 |
| 169 | 7.7452 | 0.9083 | 20.1757 | 20.83 | 33.70 |
| 283 | 4.8059 | 1.9987 | 8.5961 | 5.17 | 11.11 |
| 243 | 47.5504 | 19.7758 | 85.0510 | 130.14 | 186.70 |
| 38 | 15.4671 | 9.0398 | 23.2949 | 52.06 | 9.66 |
| 261 | 1057.0469 | 829.0645 | 1307.8988 | 2349.53 | 658.47 |

| | Proposed Bayesian Approach | | MSL-based 3 sigma (NASA Legacy) | InSight-based weighted average technique (NASA Current) |
|---|---|---|---|---|
| Component | CNI, Posterior Mean Bioburden Density – λ, CFU/$m^2$ | MOM, Posterior Mean Bioburden Density – λ, CFU/m2 | 3 sigma Bioburden Density – λ, CFU/$m^2$ | Weighted Average Bioburden Density – λ, CFU/$m^2$ |
| 9 | 2.2889 | 0.7603 | 13.84 | 27.99 |
| 73 | 0.8094 | 0.2684 | 4.87 | 17.36 |
| 300 | 2.2315 | 1.7355 | 5.96 | 9.54 |
| 169 | 7.7452 | 6.0352 | 20.83 | 33.70 |
| 283 | 4.8059 | 4.5158 | 5.17 | 11.11 |
| 243 | 47.5504 | 44.8607 | 130.14 | 186.70 |
| 38 | 15.4671 | 15.0630 | 52.06 | 9.66 |
| 261 | 1057.0469 | 1061.3672 | 2349.53 | 658.47 |

| Component # | Posterior Mean Bioburden Density – λ, CFU/$m^2$ | $5^{th}$ | $95^{th}$ | Predictive Mean, CFU | $5^{th}$ | $95^{th}$ | NASA λ, CFU/$m^2$ | NASA, CFU |
|---|---|---|---|---|---|---|---|---|
| Rollup 19 | 23.139 | 15.056 | 32.641 | 57.164 | 34 | 84 | 59.147 | 147 |
| Rollup 28 | 54.152 | 26.213 | 90.238 | 61.083 | 28 | 104 | 49.329 | 56 |
| Rollup 13 | 21.528 | 15.071 | 28.928 | 430.191 | 297 | 582 | 45.113 | 902 |

# Domination of Zero Estimator over MLE: Simulations

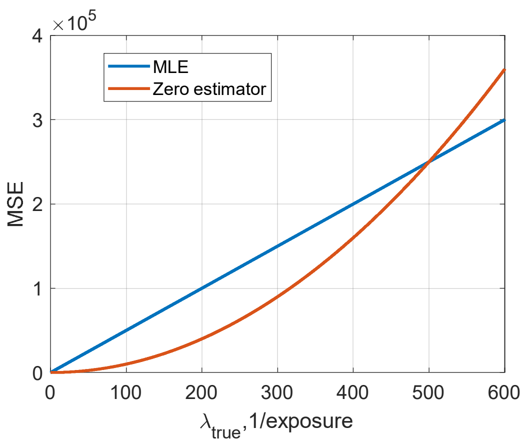
| X | e | MLE | Zero | $\lambda_{true}$ |
|---|---|---|---|---|
| 0 | 0.002 | 0 | 0 | 407.4 |
| 2 | 0.002 | 1000 | 0 | 452.9 |
| 1 | 0.002 | 500 | 0 | 63.5 |
| 2 | 0.002 | 1000 | 0 | 456.7 |
| 2 | 0.002 | 1000 | 0 | 316.2 |
| 0 | 0.002 | 0 | 0 | 48.8 |
| 0 | 0.002 | 0 | 0 | 139.2 |
| 2 | 0.002 | 1000 | 0 | 273.4 |
| 2 | 0.002 | 1000 | 0 | 478.7 |
| 2 | 0.002 | 1000 | 0 | 482.4 |

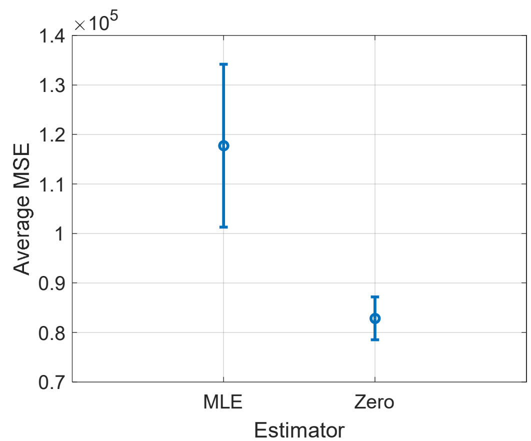



$\lambda_{true} \sim U(0,500)$

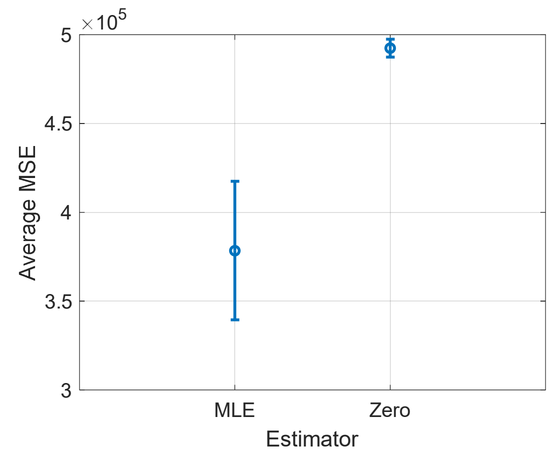
$$P(X = x|\lambda_{true}) = \frac{(\lambda_{true} \cdot e)^x}{x!} e^{-\lambda_{true} \cdot e}, x = 0,1,2, \ldots, \lambda_{true} \in (0, \infty), e \in (0, \infty)$$

# Domination of Zero Estimator over MLE: Simulations




$\lambda_{true} \sim U(0,500)$

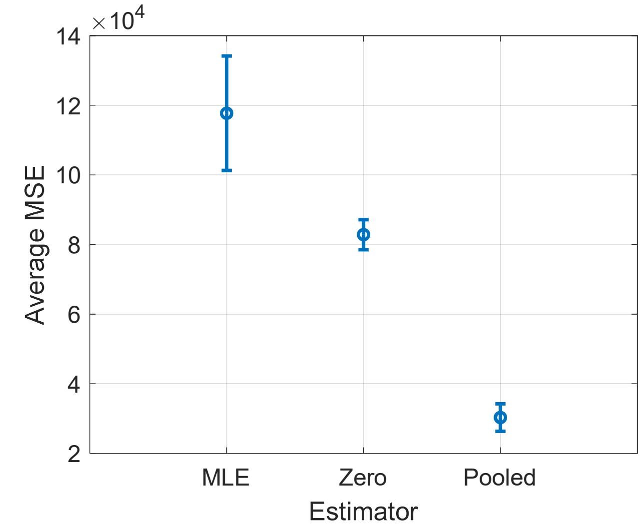



$\lambda_{true} \sim U(600,800)$

$$P(X = x|\lambda_{true}) = \frac{(\lambda_{true} \cdot e)^x}{x!} e^{-\lambda_{true} \cdot e}, x = 0,1,2, \ldots, \lambda_{true} \in (0, \infty), e \in (0, \infty)$$

# Benefits of Data Pooling

| Item Name | Sample Device | Area Sampled, $m^2$ | Pour Fraction | Exposure,$m^2$ | CFUs | Component Association |
|---|---|---|---|---|---|---|
| Cruise Stage - Outer Cylinder Section | wipe | 0.75 | 0.25 | 0.1875 | 1 | Component 300 |
| CS +Y Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| CS -Y Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| CS +X Inside | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |
| Cruise Stage - Inner Cylinder Section | wipe | 0.75 | 0.25 | 0.1875 | 0 | Component 300 |
| Cruise Stage - Cruise Stage - Inner Cylindrical Section, metal surfaces between electronic boxes | wipe | 0.75 | 0.25 | 0.1875 | 0 | Component 300 |
| CS bottom mount ring | wipe | 0.3 | 0.25 | 0.075 | 0 | Component 300 |
| Inside CS primary structure | wipe | 0.1 | 0.25 | 0.025 | 0 | Component 300 |
| Lander - Inside MLI Radar Electronics | swab | 0.0025 | 0.8 | 0.002 | 0 | Component 300 |




$$\hat{\lambda}_{MLE} = \frac{\sum_{i=1}^{N} x_i}{\sum_{i=1}^{N} e_i} \text{ ; } Maximum\ Likelihood\ Estimation\ (MLE)$$

$$MSE_{MLE} = \underbrace{E\left[\left(\hat{\lambda}_{MLE} - E\left[\hat{\lambda}_{MLE}\right]\right)^2\right]}_{Var(\hat{\lambda})} = \frac{\lambda_{true}}{\sum_{i=1}^{N} e_i}$$

# Different Losses

$Loss = (\hat{\lambda} - \lambda_{true})^2$-squared loss, minimized by conditional mean

$Loss = \frac{(\hat{\lambda} - \lambda_{true})^2}{\lambda_{true}}$ normalized squared loss, minimized by conditional mean,

$Loss = |\hat{\lambda} - \lambda_{true}|$ -absolute loss, minimized by conditional median

$$Loss = \begin{cases} a \cdot |\hat{\lambda} - \lambda_{true}| & if \ \hat{\lambda} - \lambda_{true} < 0 \\ b \cdot |\hat{\lambda} - \lambda_{true}| & if \ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases}$$

-absolute loss with different penalties for over and under estimation, minimized by a conditional quantile

$Loss = \begin{cases} 0 & if |\hat{\lambda} - \lambda_{true}| < \varepsilon \\ 1 & if |\hat{\lambda} - \lambda_{true}| \geq \varepsilon \end{cases}$ zero-one loss, minimized by maximum a posteriori (MAP)

$Loss = |\hat{\lambda} - \lambda_{true}|^p$-$L_p$ loss

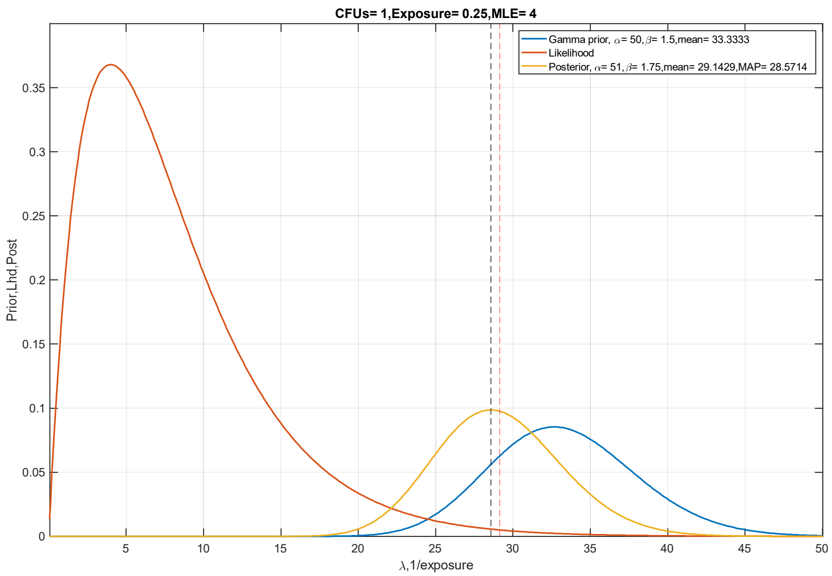
$Loss = I[|\hat{\lambda} - \lambda_{true}| > \varepsilon]$-large deviation loss

$$Loss = \begin{cases} a \cdot (\hat{\lambda} - \lambda_{true})^2 & if \ \hat{\lambda} - \lambda_{true} < 0 \\ b \cdot (\hat{\lambda} - \lambda_{true})^2 & if \ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases}$$

-squared loss with different penalties for over and under estimation, minimized by weighted conditional mean

$Loss = w(\lambda_{true}) \cdot (\hat{\lambda} - \lambda_{true})^2$-squared loss, minimized by weighted conditional mean

$$Loss = \begin{cases} 0 & if |\hat{\lambda} - \lambda_{true}| < \varepsilon \\ |\hat{\lambda} - \lambda_{true}| - \varepsilon & if \ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases} - \text{Huber } \epsilon - insensitive\ loss$$




$$MSE_{MLE} = \frac{\lambda_{true}}{e}$$

# Plots of Different Loss Functions

$Loss = (\hat{\lambda} - \lambda_{true})^2$-squared loss, minimized by conditional mean

$Loss = \frac{(\hat{\lambda} - \lambda_{true})^2}{\lambda_{true}}$- normalized squared loss, minimized by conditional mean

$Loss = |\hat{\lambda} - \lambda_{true}|$ -absolute loss, minimized by conditional median

$$Loss = \begin{cases} a \cdot |\hat{\lambda} - \lambda_{true}| & if\ \hat{\lambda} - \lambda_{true} < 0 \\ b \cdot |\hat{\lambda} - \lambda_{true}| & if\ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases}$$

-absolute loss with different penalties for over and under estimation, minimized by a conditional quantile

$Loss = \begin{cases} 0 & if |\hat{\lambda} - \lambda_{true}| < \varepsilon \\ 1 & if |\hat{\lambda} - \lambda_{true}| \geq \varepsilon \end{cases}$ zero-one loss, minimized by maximum a posteriori (MAP)

$Loss = |\hat{\lambda} - \lambda_{true}|^p$-$L_p$ loss

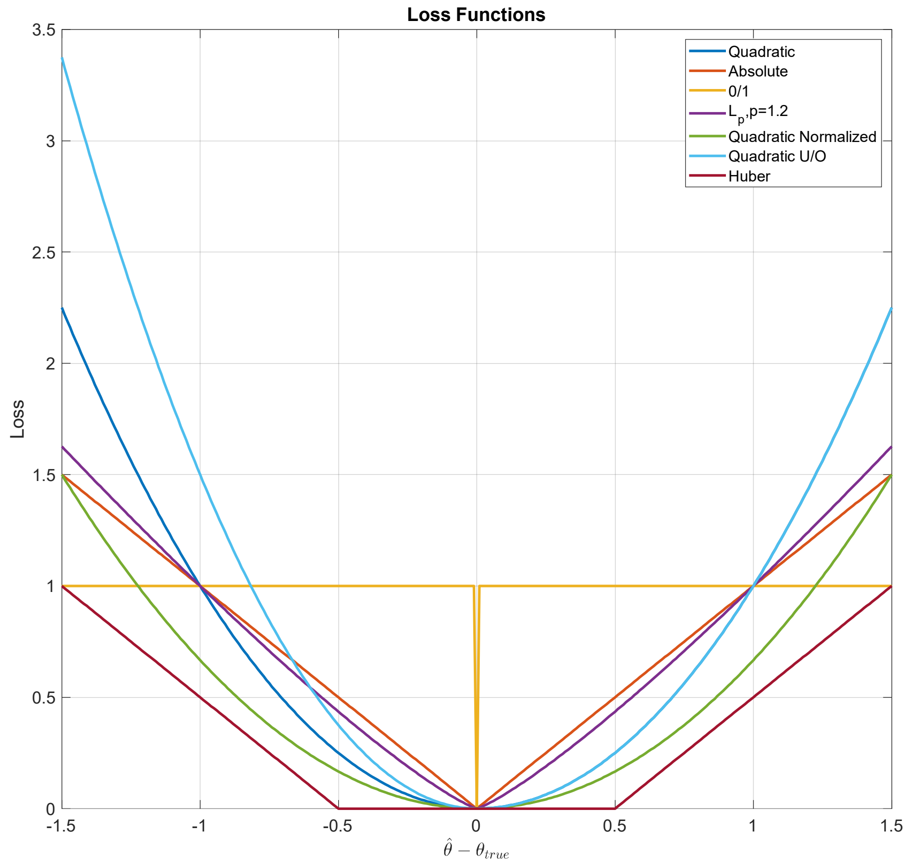
$Loss = I[|\hat{\lambda} - \lambda_{true}| > \varepsilon]$-large deviation loss

$$Loss = \begin{cases} a \cdot (\hat{\lambda} - \lambda_{true})^2 & if\ \hat{\lambda} - \lambda_{true} < 0 \\ b \cdot (\hat{\lambda} - \lambda_{true})^2 & if\ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases}$$

-squared loss with different penalties for over and under estimation, minimized by weighted conditional mean

$Loss = w(\lambda_{true}) \cdot (\hat{\lambda} - \lambda_{true})^2$-squared loss, minimized by weighted conditional mean

$$Loss = \begin{cases} 0 & if |\hat{\lambda} - \lambda_{true}| < \varepsilon \\ |\hat{\lambda} - \lambda_{true}| - \varepsilon & if\ \hat{\lambda} - \lambda_{true} \geq 0 \end{cases} - \text{Huber } \epsilon - insensitive\ loss$$



# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein)

$$E(\hat{\lambda}_{JS}|x) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\boldsymbol{\lambda})}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$B = \frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}} \le 1, \text{Variance of Gamma is inversly proportional to } \beta_{prior}$$

$$E[\hat{\lambda}_{JS}] = E\left[\left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\boldsymbol{\lambda})}\right)\right] = E\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] - B\cdot E\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] + B\cdot\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}} = \lambda_{true} - \underbrace{\left(\boldsymbol{B}\cdot\boldsymbol{\lambda_{true}} - \boldsymbol{B}\cdot\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}\right)}_{Bias}$$

$$\mathrm{Gamma}(\lambda;\alpha,\beta) = \frac{\beta^{\alpha}\cdot\lambda^{\alpha-1}\cdot e^{-\lambda\cdot\beta}}{\Gamma(\alpha)}, \alpha>0, \beta>0, \lambda\in[0,\infty]$$

$$Bias(\hat{\lambda}_{JS}) = \boldsymbol{B}\cdot\left(\boldsymbol{\lambda_{true}} - \frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}\right)$$

$$Bias(\hat{\lambda}) = E[\hat{\lambda}] - \lambda_{true} \qquad E(\lambda) = \frac{\alpha}{\beta}, Var(\lambda) = \frac{\alpha}{\beta^2}$$

$$Bias(\hat{\lambda}_{JS}) = 0 \ if \ \frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}} = \boldsymbol{\lambda_{true}}$$

$$Bias(\hat{\lambda}_{JS}) = 0 \ if \mathrm{B} = 0$$

$$\lim_{\beta_{prior}\to 0} B = \frac{\beta_{prior}}{e+\beta_{prior}} = 0 \qquad \lim_{e\to\infty} B = \frac{\beta_{prior}}{e+\beta_{prior}} = 0$$

# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein)

$$Bias(\hat{\lambda}) = E[\hat{\lambda}] - \lambda_{true}$$

$$Bias(\hat{\lambda}_{JS}) = \boldsymbol{B} \cdot \left(\boldsymbol{\lambda_{true}} - \frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}\right) \qquad B = \frac{\beta_{prior}}{\mathrm{e} + \beta_{prior}} \leq 1$$

$$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e}E[x] = \frac{1}{e} \cdot (\lambda_{true} \cdot e) = \lambda_{true}$$

$$Bias(\hat{\lambda}_{MLE}) = E[\hat{\lambda}_{MLE}] - \lambda_{true} = 0$$

# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein)

$$Var[\hat{\lambda}_{JS}] = Var\left[\left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}] \cdot \left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\boldsymbol{\lambda})}\right)\right] = Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] + B^2 \cdot Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] - 2 \cdot \rho \cdot \sqrt{Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right]} \cdot \sqrt{B^2 \cdot Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right]}$$

$$= Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] + B^2 \cdot Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] - \boldsymbol{2} \cdot \boldsymbol{B} \cdot Var\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] = \frac{\lambda_{true}}{e} + B^2 \cdot \frac{\lambda_{true}}{e} - \boldsymbol{2} \cdot \boldsymbol{B} \cdot \frac{\lambda_{true}}{e} = \frac{\lambda_{true} \cdot (1 + B^2 - \boldsymbol{2} \cdot \boldsymbol{B})}{e}$$

$$= \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}} \cdot (\boldsymbol{1} - \boldsymbol{B})^{\boldsymbol{2}}$$

$$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2} Var[x] = \frac{1}{e^2} \cdot (\lambda_{true} \cdot e) = \frac{\lambda_{true}}{e}$$

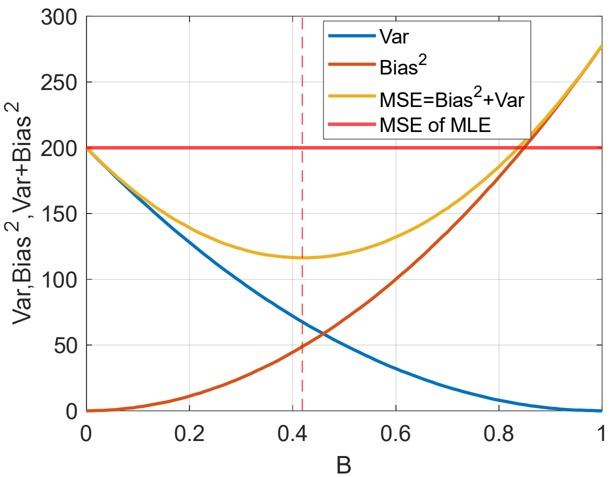
$$Var[\hat{\lambda}_{JS}] = \frac{\lambda_{true}}{e} \cdot (1 - B)^2 \leq Var[\hat{\lambda}_{MLE}] = \frac{\lambda_{true}}{e} \qquad B = \frac{\beta_{prior}}{\mathrm{e} + \beta_{prior}} \leq 1$$

$$Var[\hat{\lambda}_{JS}] = Var[\hat{\lambda}_{MLE}] = \frac{\lambda_{true}}{e}, if\ B = 0 \qquad Var[\hat{\lambda}_{JS}] = 0, if\ B = 1$$

# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein)

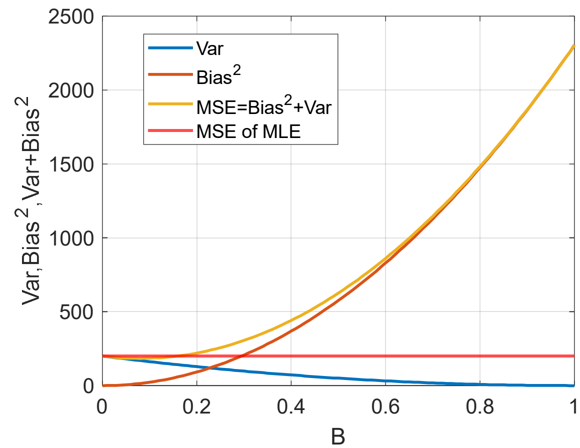
$$MSE_{JS} = \underbrace{E\left[(\hat{\lambda}_{JS} - E[\hat{\lambda}_{JS}])^2\right]}_{Var(\hat{\lambda})} + \underbrace{\left(E[\hat{\lambda}_{JS}] - \lambda_{true}\right)^2}_{Bias(\hat{\lambda})^2}$$

$$MSE_{JS} = \frac{\lambda_{true}}{e} \cdot (1-B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$$



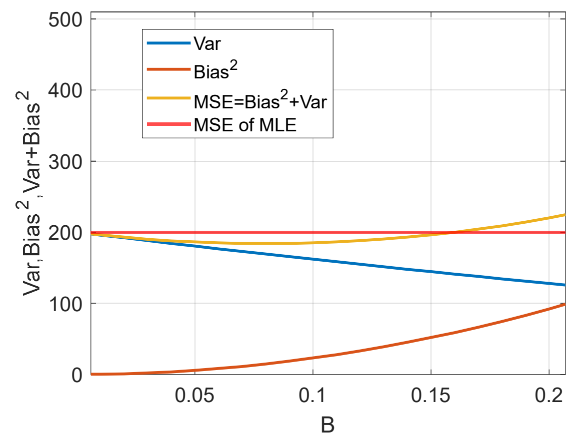

$$\frac{\alpha_{prior}}{\beta_{prior}} = 33.3\ \text{CFUs}/m^2$$

$$\lambda_{true} = 50\ \text{CFUs}/m^2$$




$$\frac{\alpha_{prior}}{\beta_{prior}} = 2\ \text{CFUs}/m^2$$

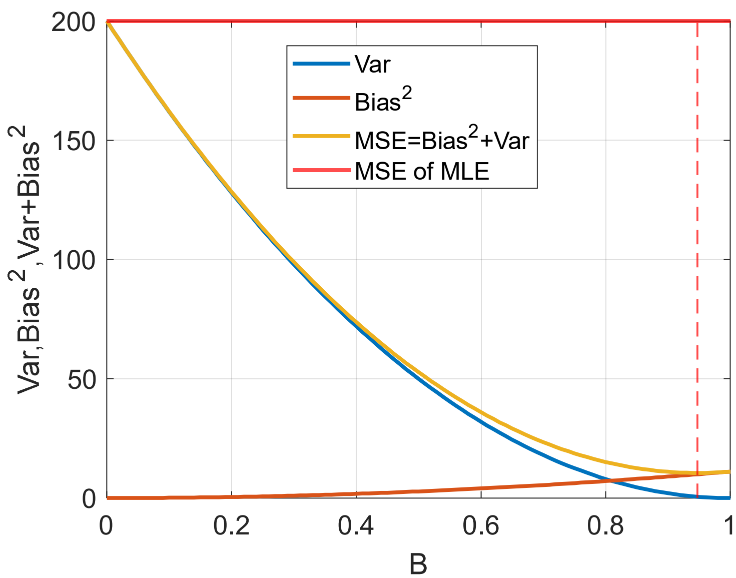
$$\lambda_{true} = 50\ \text{CFUs}/m^2$$




$$B = \frac{\beta_{prior}}{e + \beta_{prior}} \leq 1$$

# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein)

$$MSE_{JS} = \frac{\lambda_{true}}{e} \cdot (1 - B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$$




$$\frac{\alpha_{prior}}{\beta_{prior}} = 46.6 \text{ CFUs}/m^2$$

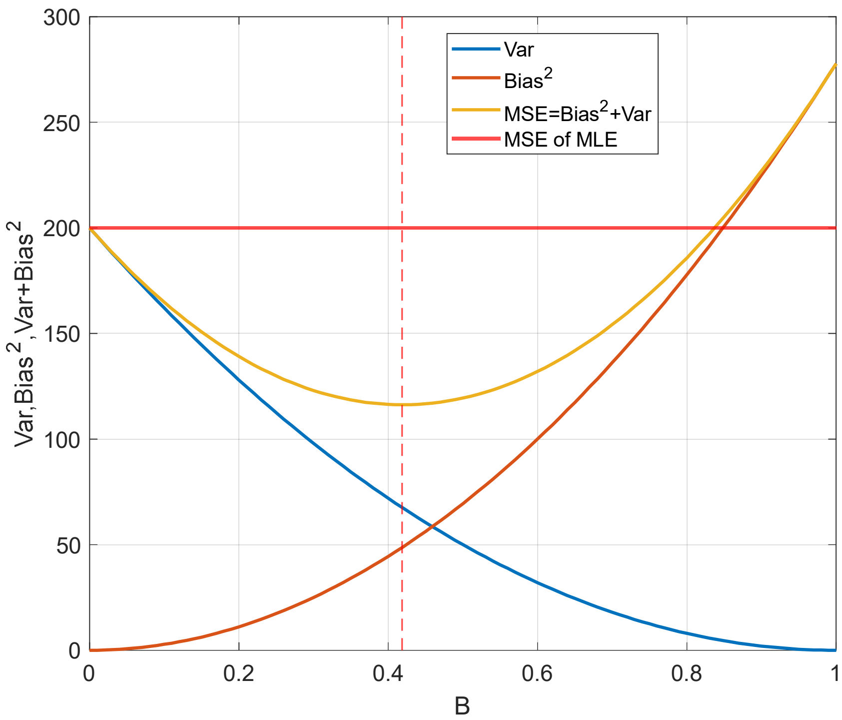
$$\lambda_{true} = 50 \text{ CFUs}/m^2$$

# Borrowing Information

$$E\left(\hat{\lambda}_{JS}\middle|x\right) = [1-B]\cdot\left(\frac{x}{e}\right) + [B]\cdot\left(\frac{\alpha_{prior}}{\beta_{prior}}\right) = \left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}]\cdot\left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{E_{prior}}(\boldsymbol{\lambda})}\right) = \left(\frac{x}{e}\right) - \left[\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}\right]\cdot\left(\frac{x}{e} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$\frac{\alpha_{prior}}{\beta_{prior}} = 33.3\ \text{CFUs}/m^2$$

$$\lambda_{true} = 50\ \text{CFUs}/m^2$$



# Bias-Variance Decomposition-Posterior Mean Estimator (James-Stein). Shrinking towards zero

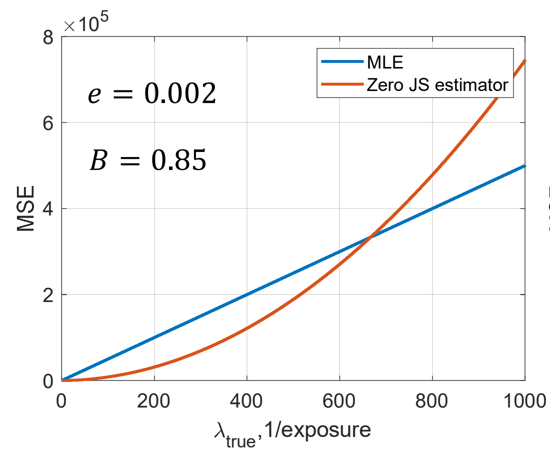
$$E[\hat{\lambda}_{JS(0)}] = E\left[\left(\frac{\boldsymbol{x}}{\boldsymbol{e}}\right) - [\boldsymbol{B}] \cdot \left(\frac{\boldsymbol{x}}{\boldsymbol{e}} - \underbrace{\frac{\boldsymbol{\alpha_{prior}}}{\boldsymbol{\beta_{prior}}}}_{\boldsymbol{0}}\right)\right] = E\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] - B \cdot E\left[\frac{\boldsymbol{x}}{\boldsymbol{e}}\right] = \lambda_{true} - \underbrace{(\boldsymbol{B} \cdot \boldsymbol{\lambda_{true}})}_{Bias}$$

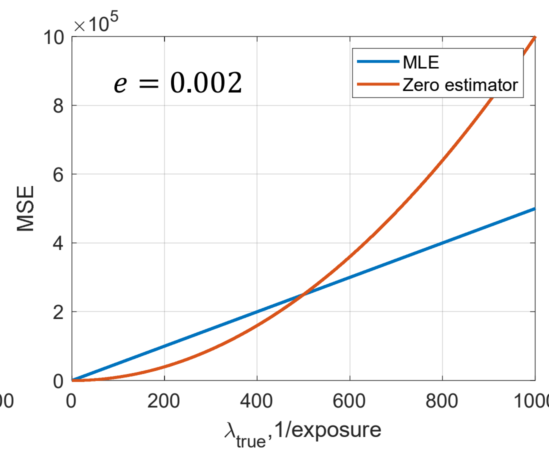
$$Var[\hat{\lambda}_{JS(0)}] = \frac{\lambda_{true}}{e} \cdot (1 - B)^2$$

$$MSE_{JS(0)} = \frac{\lambda_{true}}{e} \cdot (1 - B)^2 + (-B \cdot \lambda_{true})^2$$

$$MSE_0 = \lambda_{true}{}^2 \qquad B = \frac{\beta_{prior}}{\mathrm{e} + \beta_{prior}} \leq 1$$

$\lambda_{true} = 50 \text{ CFUs}/m^2$



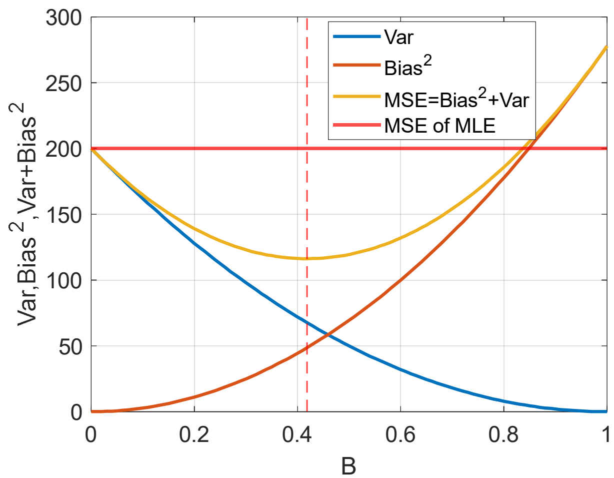

$$\text{Gamma}(\lambda; \alpha, \beta) = \frac{\beta^{\alpha} . \lambda^{\alpha - 1} . e^{-\lambda \cdot \beta}}{\Gamma(\alpha)}, \alpha > 0, \beta > 0, \lambda \in [0, \infty]$$

# Optimal Parameter B

$$MSE_{JS} = \frac{\lambda_{true}}{e} \cdot (1 - B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$$

$$\frac{dMSE_{JS}}{dB} = 0$$

$$B_{opt} = \frac{\frac{\lambda_{true}}{e}}{\frac{\lambda_{true}}{e} + \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)^2}$$

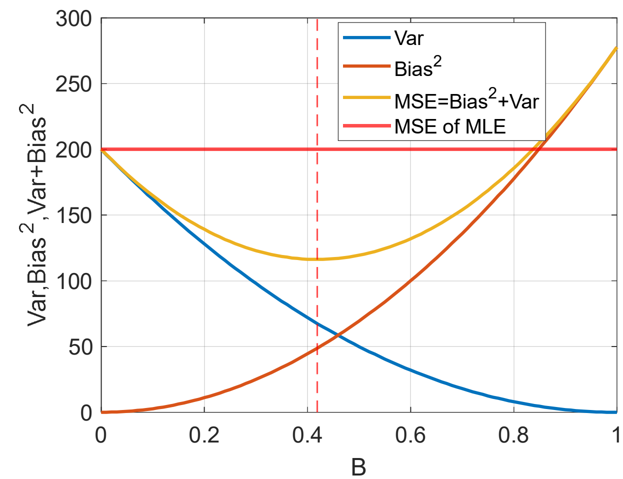


# Bias-Variance for Different Priors

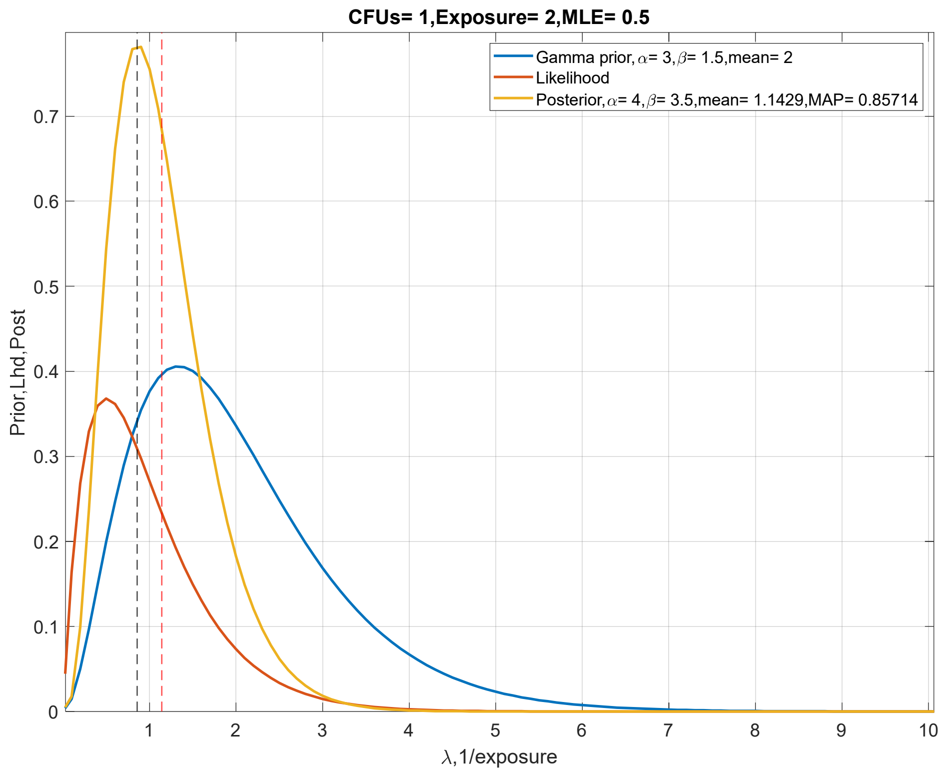
| Prior | α,β | Bias($\hat{\lambda}$) | Var($\hat{\lambda}$) |
| --- | --- | --- | --- |
| Jeffreys | Gamma(0.5,0)-improper prior | $\lim_{\beta_{prior}\to 0} \frac{\beta_{prior}}{e+\beta_{prior}} \cdot \left(\lambda_{true} - \frac{0.5}{\beta_{prior}}\right)$ | $\lim_{\beta_{prior}\to 0} \frac{\lambda_{true}}{e} \cdot \left(1 - \frac{\beta_{prior}}{e+\beta_{prior}}\right)^2$ |
| Uniform | Gamma(1,0) | $\frac{x+\alpha}{e+\beta} = \frac{x}{e} + \frac{1}{e}$ | $\frac{1}{e}$ |
| Max Entropy | Gamma(1,1/μ) | $\frac{\mu(x+1)}{e\cdot\mu+1}$ | $\frac{\mu}{e\cdot\mu+1}$ |
| Constrained noninformative (CNI) | Gamma(0.5, 1/(2·μ)) | $\frac{2\cdot\mu(x+0.5)}{2\cdot e\cdot\mu+1}$ | $\frac{\mu}{2\cdot e\cdot\mu+1}$ |
| Gamma prior | Gamma(α, β) | $\frac{x+\alpha}{e+\beta}$ | $\frac{\alpha}{e+\beta}$ |
| | | | |

$$MSE_{JS} = \frac{\lambda_{true}}{e} \cdot (1-B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$$

$$B = \frac{\beta_{prior}}{e+\beta_{prior}} \le 1$$



# Maximum A Posteriori (MAP) estimate




$$E_{post}(\lambda|x) = \frac{x + \alpha_{prior}}{\mathrm{e} + \beta_{prior}}$$

$$\mathrm{Mode}(\lambda|x) = \frac{x+\alpha_{prior}-1}{\mathrm{e}+\beta_{prior}} \qquad x + \alpha_{prior} \geq 1$$

$$\mathrm{Mode}(\hat{\lambda}_{MAP}|x) = \frac{x+\alpha_{prior}-1}{\mathrm{e}+\beta_{prior}} = \left[\frac{e}{\mathrm{e}+\beta_{prior}}\right] \cdot \left(\frac{x-1}{e}\right) + \left[\underbrace{\frac{\beta_{prior}}{\mathrm{e}+\beta_{prior}}}_{B}\right] \cdot \left(\frac{\alpha_{prior}}{\beta_{prior}}\right)$$

$$Bias(\hat{\lambda}_{MAP}) = B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right) + \frac{1-B}{e}$$

$$Bias(\hat{\lambda}_{JS}) = B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$$

# Parameter Estimators

| Estimator | Bias | Variance | MSE | B, optimal |
|---|---|---|---|---|
| MLE | 0 | $\frac{\lambda_{true}}{e}$ | $\frac{\lambda_{true}}{e}$ | N/A |
| Zero | ${\lambda_{true}}^2$ | 0 | ${\lambda_{true}}^2$ | N/A |
| EB-JS, zero prior mean | $B \cdot \lambda_{true}$ | $\frac{\lambda_{true}}{e} \cdot (1-B)^2$ | $\frac{\lambda_{true}}{e} \cdot (1-B)^2 + (-B \cdot \lambda_{true})^2$ | $\frac{\frac{\lambda_{true}}{e}}{\frac{\lambda_{true}}{e} + {\lambda_{true}}^2}$ |
| EB-JS | $B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)$ | $\frac{\lambda_{true}}{e} \cdot (1-B)^2$ | $\frac{\lambda_{true}}{e} \cdot (1-B)^2 + \left(B \cdot \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)\right)^2$ | $\frac{\frac{\lambda_{true}}{e}}{\frac{\lambda_{true}}{e} + \left(\lambda_{true} - \frac{\alpha_{prior}}{\beta_{prior}}\right)^2}$ |
| MAP | | | | |
| Clevenson-Zidek (CZ) | | | | |

# Recovery Efficiency Model as Shrinkage Estimator

$$P(X = x|\lambda_{true}) = \frac{(\lambda_{true} \cdot e)^x}{x!} e^{-\lambda_{true} \cdot e}, x = 0,1,2, \ldots, \lambda_{true} \in (0, \infty), e \in (0, \infty)$$

*x-CFU counts*
*λ- bioburden density, CFUs/m²*
*e- exposure, pour ratio*area sampled, m²*

$$E[X] = \lambda_{true} \cdot e, Var[X] = \lambda_{true} \cdot e$$

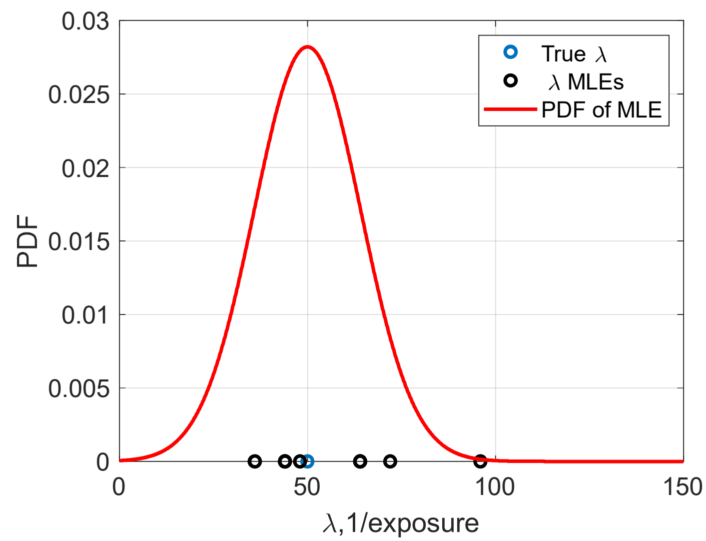
$$\hat{\lambda}_{MLE} = \frac{x}{e}\ ; Maximum\ Likelihood\ Estimation\ (MLE) \qquad \hat{\lambda}_{MLE} = \frac{x + \epsilon}{e}$$

$$E[\hat{\lambda}_{MLE}] = E\left[\frac{x}{e}\right] = \frac{1}{e} E[x] = \frac{1}{e} \cdot (\lambda_{true} \cdot e) = \lambda_{true}$$

$$Var[\hat{\lambda}_{MLE}] = Var\left[\frac{x}{e}\right] = \frac{1}{e^2} Var[x] = \frac{1}{e^2} \cdot (\lambda_{true} \cdot e) = \frac{\lambda_{true}}{e}$$

$$Loss = \left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right], Squared\ difference$$

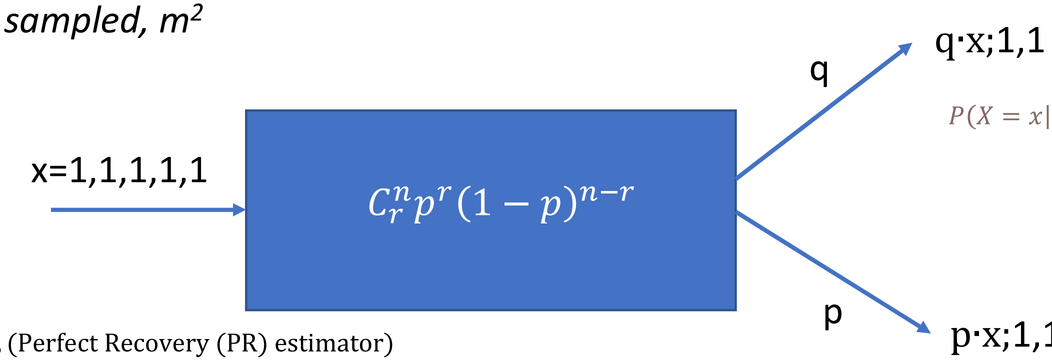
$$Risk = MSE = E\left[(\hat{\lambda}_{MLE} - \lambda_{true})^2\right], Mean\ Squared\ Error\ (MSE)$$



# Recovery Efficiency (RE) and Measurement's noise (systematic and random errors)

*x-CFU counts*
*λ- bioburden density, CFUs/m²*
*e- exposure, pour ratio*area sampled, m²*

$$P(X = x|\lambda_{true}) = \frac{(\lambda_{true} \cdot e)^x}{x!} e^{-\lambda_{true} \cdot e},$$
$$x = 0,1,2,\ldots, \lambda_{true} \in (0,\infty), \text{e} \in (0,\infty)$$




$$P(X = x|q \cdot \lambda_{true}) = \frac{(q \cdot \lambda_{true} \cdot e)^x}{x!} e^{-q \cdot \lambda_{true} \cdot e},$$

$$P(X = x|p \cdot \lambda_{true}) = \frac{(p \cdot \lambda_{true} \cdot e)^x}{x!} e^{-p \cdot \lambda_{true} \cdot e},$$

$$\hat{\lambda}_{MLE}^{PR} = \frac{x + alfa}{e + beta}, assumes\ perfect\ recovery, \text{(Perfect Recovery (PR) estimator)}$$

$$\hat{\lambda}_{MLE}^{RE} = \frac{x - \epsilon + alfa}{e + beta}, = \frac{x}{e} \cdot p, assumes\ partial\ recovery, (Recovery\ Efficiency (RE)\ estimator)$$

$$\hat{\lambda}_0 = 0, assumes\ no\ recovery, (Zero\ estimator)$$

p-probability of keeping a CFU count (efficiency)
q=(1-p)-probability of deleting a CFU count (1-efficiency)

$$Risk = MSE = E\left[(\hat{\lambda} - \lambda_{true})^2\right], \boldsymbol{Symmetric}\ Mean\ Squared\ Error\ (MSE)$$

# Bias and Variance of the RE estimator

$$E[\hat{\lambda}_{MLE}^{RE}] = E\left[\frac{x-\varepsilon}{e}\right] = \frac{1}{e}E[x-\varepsilon] = \frac{1}{e}\cdot(\lambda_{true}\cdot\varepsilon) - E(\varepsilon) = \lambda_{true} - \lambda_{true}\cdot \mathrm{q} = \lambda_{true}\cdot(1-\mathrm{q}) = \lambda_{true}\cdot p$$

$$Bias[\hat{\lambda}_{MLE}^{RE}] = \lambda_{true} - \lambda_{true}\cdot \mathrm{q} - \lambda_{true} = -\boldsymbol{\lambda_{true}}\cdot\mathbf{q}$$

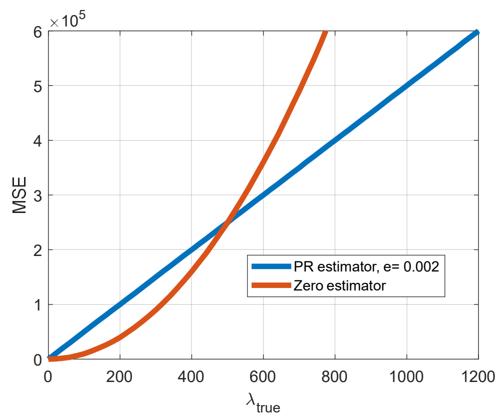
$$Var[\hat{\lambda}_{MLE}^{RE}] = Var\left[\frac{x-\epsilon}{e}\right] = \frac{1}{e^2}Var[x-\epsilon] = Var\left[\frac{x}{e}\right] + Var\left[\frac{\epsilon}{e}\right] - 2\cdot Cov\left(\frac{x}{e},\frac{\varepsilon}{e}\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(E\left[\frac{x}{e}\cdot\frac{q\cdot x}{e}\right] - E\left[\frac{x}{e}\right]\cdot E\left[\frac{q\cdot x}{e}\right]\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(q\cdot E\left[\frac{x}{e}\cdot\frac{x}{e}\right] - q\cdot E\left[\frac{x}{e}\right]\cdot E\left[\frac{x}{e}\right]\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot\left(q\cdot E\left[\left(\frac{x}{e}\right)^2\right] - q\cdot\left(E\left[\frac{x}{e}\right]\right)^2\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\left(E\left[\left(\frac{x}{e}\right)^2\right] - \left(E\left[\frac{x}{e}\right]\right)^2\right) = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\cdot Var\left[\frac{x}{e}\right] = \frac{\lambda_{true}}{e} + \frac{\lambda_{true}}{e}\cdot q^2 - 2\cdot q\cdot\frac{\lambda_{true}}{e} = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1} + q^2 - \mathbf{2}\cdot\boldsymbol{q}) = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot\boldsymbol{p}^{\mathbf{2}}$$

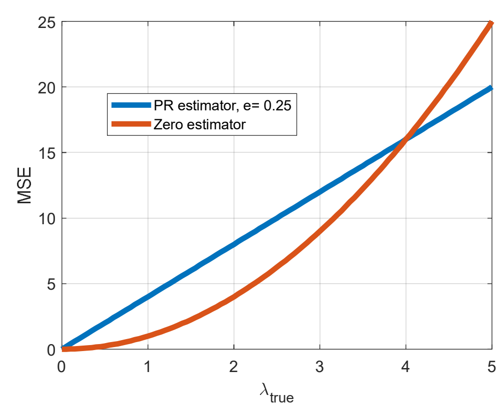
$$MSE(\hat{\lambda}_{MLE}^{RE}) = Bias^2 + Var = (-\boldsymbol{\lambda_{true}}\cdot\mathbf{q})^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = (-\boldsymbol{\lambda_{true}}\cdot(\mathbf{1}-\boldsymbol{p}))^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}}\cdot\boldsymbol{p}^{\mathbf{2}}$$

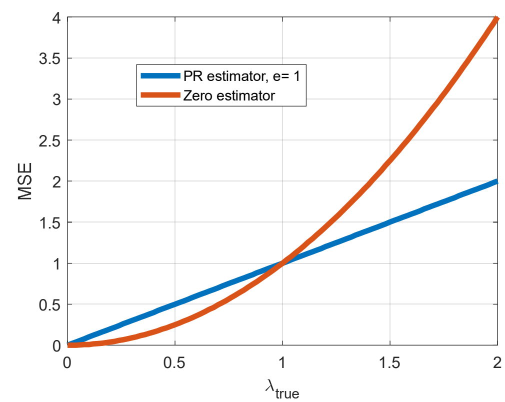
# MSE of the Recover Efficiency for Symmetric Penalty Function

$$MSE(\hat{\lambda}_{MLE}^{RE}) = Bias^2 + Var = (-\boldsymbol{\lambda}_{true}\cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda}_{true}}{\boldsymbol{e}}\cdot(\mathbf{1}-\boldsymbol{q})^{\mathbf{2}} = (-\boldsymbol{\lambda}_{true}\cdot(\mathbf{1}-\boldsymbol{p}))^2 + \frac{\boldsymbol{\lambda}_{true}}{\boldsymbol{e}}\cdot \boldsymbol{p}^{\mathbf{2}}$$

$$MSE(\hat{\lambda}_{MLE}^{PR}) = \frac{\lambda_{true}}{e}, p = 1 \qquad MSE_0 = {\lambda_{true}}^2, p = 0 \qquad \lambda_{true} < \frac{1}{e}$$



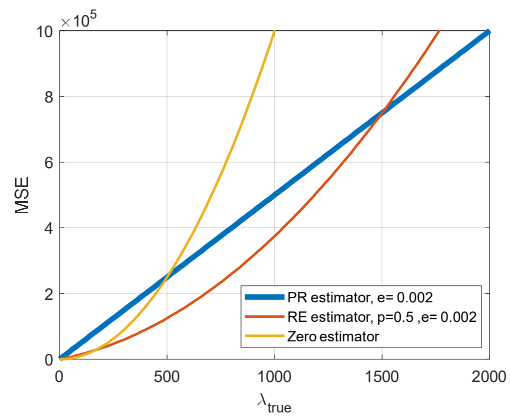



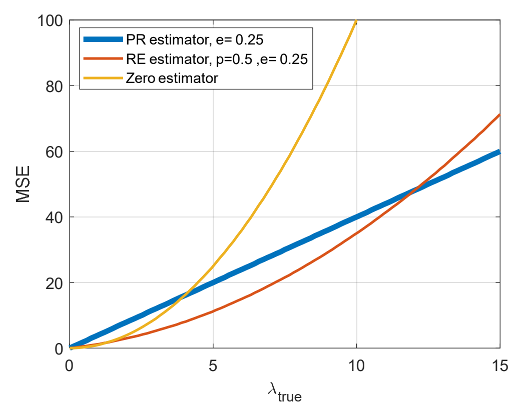



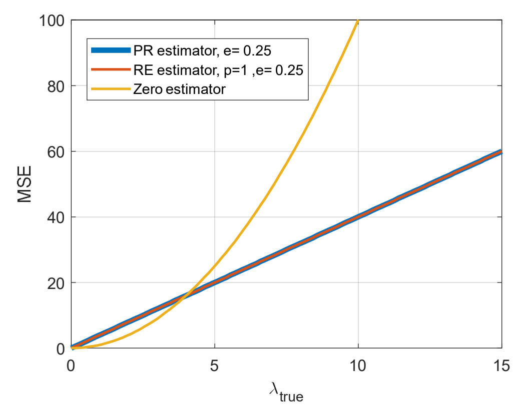

Zero estimator (p=0) will dominate PR estimator (p=1) up to the values of $\lambda_{true}$ <1/e

# MSE of the Recovery Efficiency Model as a Function of $\boldsymbol{\lambda_{true}}$

$$MSE(\hat{\lambda}_{MLE}^{RE}) = Bias^2 + Var = (-\boldsymbol{\lambda_{true}} \cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}} \cdot (\mathbf{1} - \boldsymbol{q})^2 = (-\boldsymbol{\lambda_{true}} \cdot (\mathbf{1} - \boldsymbol{p}))^2 + \frac{\lambda_{true}}{e} \cdot \boldsymbol{p}^2$$

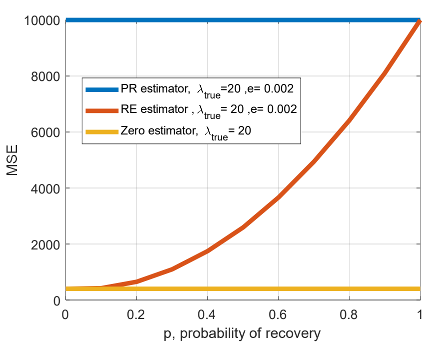


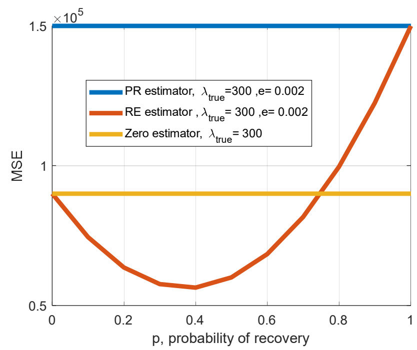



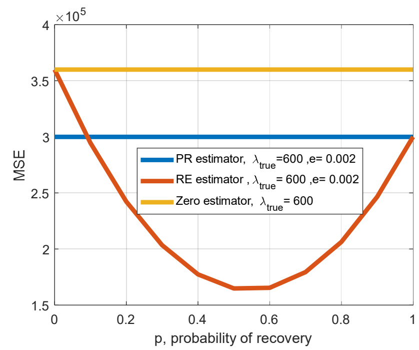



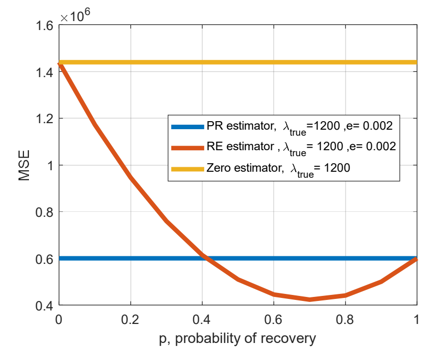

RE estimator (0<p<1) will dominate PR estimator (p=1) up to the values of $\lambda_{true} < \frac{(1-p)}{e \cdot (1-p)}$, RE estimator will dominate Zero estimator (p=0) for $\lambda_{true} > \frac{p}{e \cdot (2-p)}$ . In addition, for $\lambda_{true} < \frac{p}{e \cdot (2-p)}$ , Zero estimator will dominate both RE and PR estimator

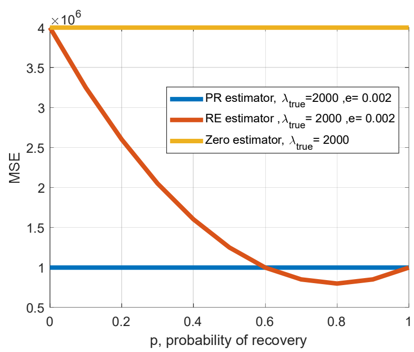
# MSE of the Recovery Efficiency Model as a Function of p for swab exposure



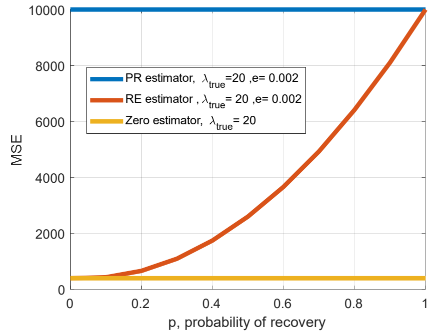



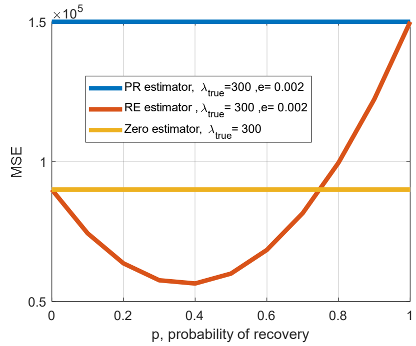



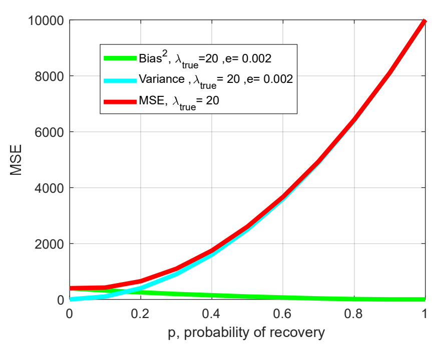

$$MSE(\hat{\lambda}_{MLE}^{RE}) = Bias^2 + Var = (-\boldsymbol{\lambda_{true}}\cdot \mathbf{q})^2 + \frac{\boldsymbol{\lambda_{true}}}{\boldsymbol{e}} \cdot (\mathbf{1} - \boldsymbol{q}) = (-\boldsymbol{\lambda_{true}}\cdot (\mathbf{1} - \boldsymbol{p}))^2 + \frac{\lambda_{true}}{e} \cdot \boldsymbol{p^2}$$

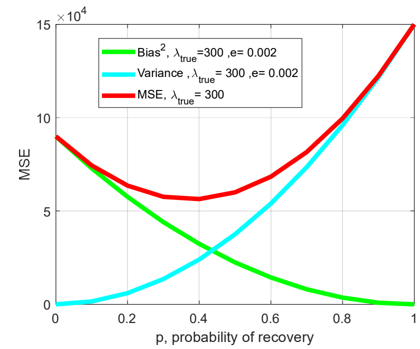
# Bias-Variance Decomposition of the RE estimator



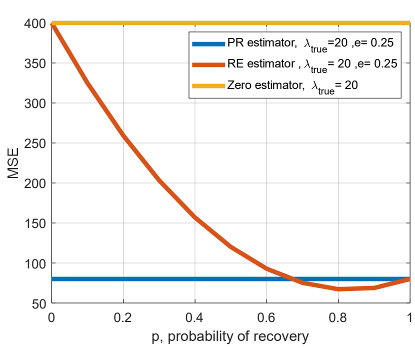

$$\hat{\lambda}_{MLE}^{PR} = \frac{1}{0.002} = 500\ CFUs/m^2$$

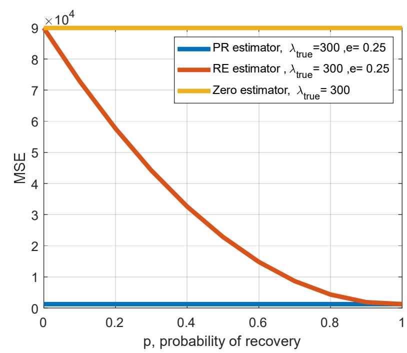


# MSE of the Recovery Efficiency Model as a Function of p for wipe exposure

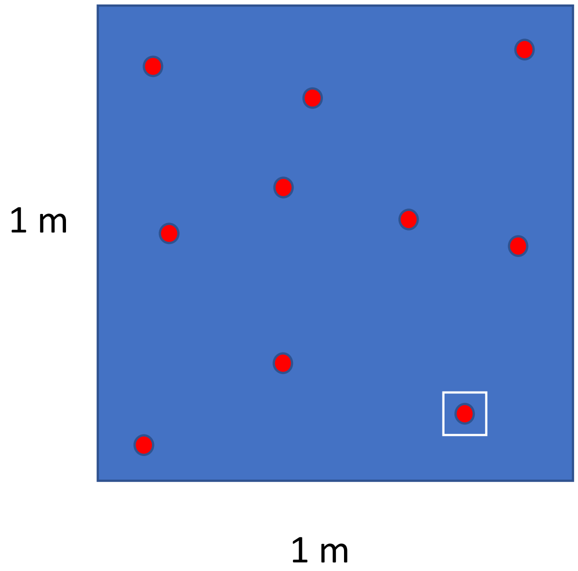



$$MSE(\hat{\lambda}^{RE}_{MLE}) = (-\lambda_{true}\cdot(1-p))^2 + \frac{\lambda_{true}}{e}\cdot p^2$$

- The RE estimator is a compromise between perfect recovery estimator and zero estimator
- RE estimator (0<p<1) will dominate PR estimator (RE=1,p=1) up to the values of $\lambda_{true} < \frac{(1-p)}{e\cdot(1-p)}$
- The degree of domination is a function of p and e
- For small e=0.002 (swab), and small $\lambda_{true}$ , the domination is guaranteed for any value of efficiency p.
- As $\lambda_{true}$ increases, $MSE(\hat{\lambda}^{RE}_{MLE})$shows a minimal value which is reached for optimal p
- For further increase in $\lambda_{true}$ the optimal value still exists , however there a minimal value of p below which the RE estimator no longer dominates the PR estimator
- For large e≥0.25, the influence of recovery efficiency is significantly more prominent (decisive actually) as even for small $\lambda_{true}$ , the efficiency needs to be nearly 1 to approach the PR estimator
- The RE estimator performs as a shrinkage estimator, as it shrinks variance of the estimate at the expense of introducing bias
- This may lead to a better estimate that the perfect recovery estimator

# Zero Estimator vs MLE




$$\lambda_{true} = 10\ \frac{CFU}{m^2}$$

$$L = (0 - \lambda_{true})^2 = (0 - 10)^2 = 10^2 = 100;\ \sqrt{100} = 10\ \frac{CFU}{m^2}$$

$$\hat{\lambda} = \frac{1}{0.0025\ m^2} = 400\,\frac{CFUs}{m^2}$$

$$L = (400 - \lambda_{true})^2 = (400 - 10)^2 = 390^2 = 152100;\ \sqrt{152100} = 390\ \frac{CFU}{m^2}$$

$$P_{CFU} = \frac{10}{400};\, P_{NO\ CFU} = \frac{390}{400}$$

$$L = \frac{10}{400} \cdot 390 + \frac{390}{400} \cdot 10 = \frac{1}{4} \cdot 39 + \frac{39}{4} \cdot 1 = \frac{39}{4} + \frac{39}{4} = \frac{39 + 39}{4} = \frac{78}{4} = 19.5\ \frac{CFU}{m^2}$$

# Technical Update Briefing Outline

- Selection of the cost function for estimating bioburden density
- Design of sampling strategies for estimating bioburden density
- Bayesian risk for different estimators
- Integration of efficiency model in Bayesian bioburden density estimation model

# Risks of the Deterministic Estimator

$$Risk_{Freq}\left(\lambda_{true}, \hat{\lambda}(x)\right) = \sum_{x=0}^{\infty} \left(\hat{\lambda}(x) - \lambda_{true}\right)^2 \cdot \frac{(\lambda_{true} \cdot ex)^x}{x!} \cdot e^{-\lambda_{true} \cdot ex}$$

$$Risk_{Freq}(\lambda_{true}, d\ ) = \sum_{x=0}^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot \frac{(\lambda_{true} \cdot ex)^x}{x!} \cdot e^{-\lambda_{true} \cdot ex} = \sum_{x=0}^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot Poisson(x|\lambda_{true}) = \sum_{x=0}^{\infty} \left(\mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2\right) \cdot Poisson(x|\lambda_{true}) =$$

$$= \sum_{x=0}^{\infty} \mathrm{d}^2 \cdot Poisson(x|\lambda_{true}) - 2 \cdot d \cdot \lambda_{true} \cdot \sum_{x=0}^{\infty} Poisson(x|\lambda_{true}) + {\lambda_{true}}^2 \cdot \sum_{x=0}^{\infty} Poisson(x|\lambda_{true}) = \mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2 = (\mathrm{d} - \lambda_{true})^2$$

$$Risk_{Int}(\lambda_{true}, d\ ) = \int_0^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) d\lambda_{true} = \int_0^{\infty} \left(\mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2\right) \cdot Gamma(\lambda_{true}|\alpha, \beta) d\lambda_{true} =$$

$$= \int_0^{\infty} \mathrm{d}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) d\lambda_{true} - 2 \cdot d \cdot \int_0^{\infty} \lambda_{true} \cdot Gamma(\lambda_{true}|\alpha, \beta) d\lambda_{true} + \int_0^{\infty} {\lambda_{true}}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) d\lambda_{true} =$$

$$= \mathrm{d}^2 - 2 \cdot d \cdot \frac{\alpha}{\beta} + \frac{\alpha + \alpha^2}{\beta^2} = \left[d - \frac{\alpha}{\beta}\right]^2 + \frac{\alpha}{\beta^2}$$

$$E\left({\lambda_{true}}^2\right) = Var(\lambda_{true}) + [E(\lambda_{true})]^2 = \frac{\alpha}{\beta^2} + \left[\frac{\alpha}{\beta}\right]^2$$

$$Gamma(\lambda_{true}|\alpha, \beta) = \frac{\beta^{\alpha} \cdot \lambda_{true}^{\alpha-1} \cdot e^{-\lambda_{true} \cdot \beta}}{\Gamma(\alpha)}$$

# Risks of the Deterministic Estimator

$$Risk_{Freq}(\lambda_{true}, d) = \sum_{x=0}^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot \frac{(\lambda_{true} \cdot ex)^x}{x!} \cdot e^{-\lambda_{true} \cdot ex} = \sum_{x=0}^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot Poisson(x|\lambda_{true}) = \sum_{x=0}^{\infty} \left(\mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2\right) \cdot Poisson(x|\lambda_{true}) =$$

$$= \sum_{x=0}^{\infty} \mathrm{d}^2 \cdot Poisson(x|\lambda_{true}) - 2 \cdot d \cdot \lambda_{true} \cdot \sum_{x=0}^{\infty} Poisson(x|\lambda_{true}) + {\lambda_{true}}^2 \cdot \sum_{x=0}^{\infty} Poisson(x|\lambda_{true}) = \mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2 = (\mathrm{d} - \lambda_{true})^2$$

$$Risk_{Int}(\lambda_{true}, d) = \int_0^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) = \int_0^{\infty} \left(\mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2\right) \cdot Gamma(\lambda_{true}|\alpha, \beta) =$$

$$= \int_0^{\infty} \mathrm{d}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) - 2 \cdot d \cdot \int_0^{\infty} \lambda_{true} \cdot Gamma(\lambda_{true}|\alpha, \beta) + \int_0^{\infty} {\lambda_{true}}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) =$$

$$= \mathrm{d}^2 - 2 \cdot d \cdot \frac{\alpha}{\beta} + \frac{\alpha + \alpha^2}{\beta^2} = \left[d - \frac{\alpha}{\beta}\right]^2 + \frac{\alpha}{\beta^2}$$

$$Risk_{Bayes}(\lambda_{true}, d) = \int_0^{\infty} (\mathrm{d} - \lambda_{true})^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) = \int_0^{\infty} \left(\mathrm{d}^2 - 2 \cdot d \cdot \lambda_{true} + {\lambda_{true}}^2\right) \cdot Gamma(\lambda_{true}|\alpha, \beta) =$$

$$= \int_0^{\infty} \mathrm{d}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) - 2 \cdot d \cdot \int_0^{\infty} \lambda_{true} \cdot Gamma(\lambda_{true}|\alpha, \beta) + \int_0^{\infty} {\lambda_{true}}^2 \cdot Gamma(\lambda_{true}|\alpha, \beta) =$$

$$= \mathrm{d}^2 - 2 \cdot d \cdot \frac{\alpha}{\beta} + \frac{\alpha + \alpha^2}{\beta^2} = \left[d - \frac{\alpha}{\beta}\right]^2 + \frac{\alpha}{\beta^2}$$