Bayesian Elegance in Resolving Semiconductor Manufacturing Challenges

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Presented at Lam Research Webminar, Jan 25, 2024

Semiconductor Manufacturing

Problems: yield estimation, recipe optimization, process control, variation analysis,…

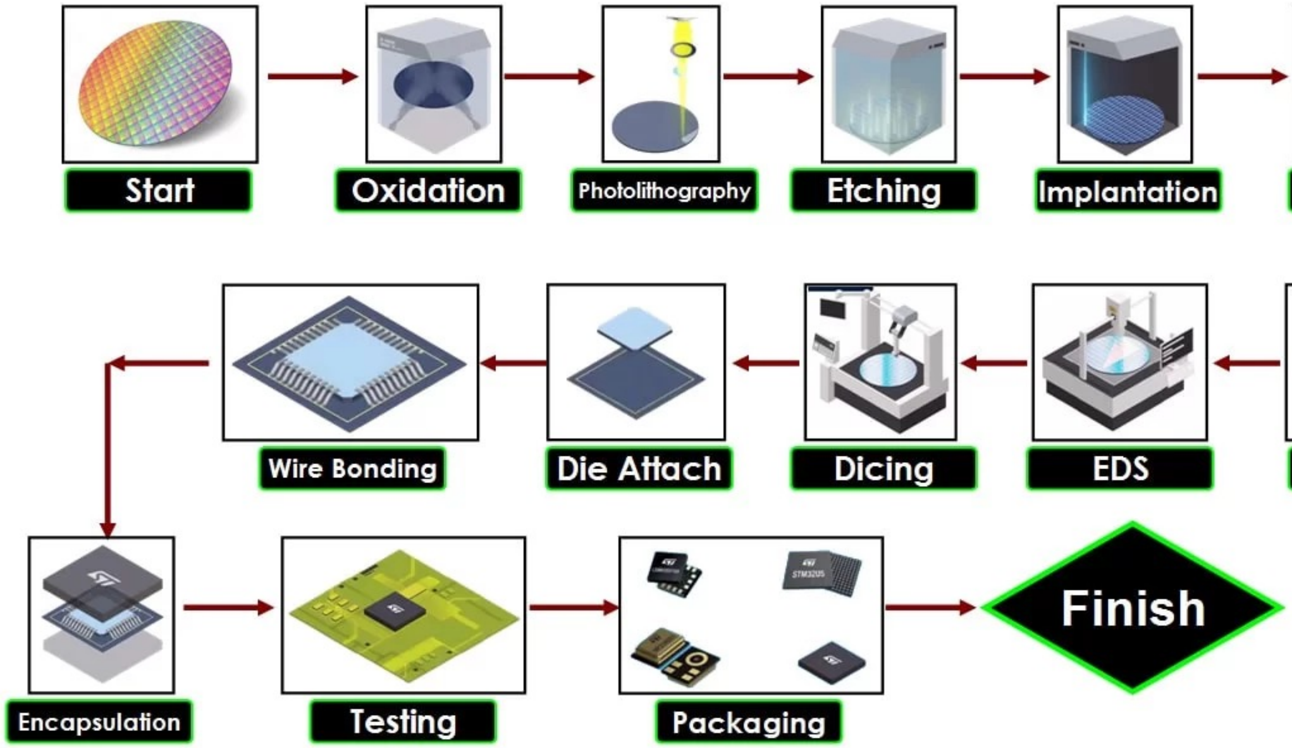

Figure Credit: https://shorturl.at/uBFH1

Three Characteristics of Semiconductor Manufacturing Problems

- **Fact 1: Costly function evaluation (usually black-box)**
  - Simulators (COMSOL, Coventor Products, SPICE, etc.,) usually run slowly
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  - Algorithms asymptotic performances rely on the amount of data
  - Fewer data, less accurate (e.g., regression accuracy)
- **Fact 3: Intricate correlations among various scenarios**
  - Early-stage and late-stage correlations (e.g., front-end and back-end)
  - Multiple-corner correlations (e.g., {SS, TT, FF, SF, FS} process corners)

Three Characteristics of Semiconductor Manufacturing Problems

- Aim for a framework
  - Only assumes black-box function
  - Work with limited data
  - Can easily embed human knowledge

Bayesian Method: $$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)} \propto P(B|A)\,P(A)$$

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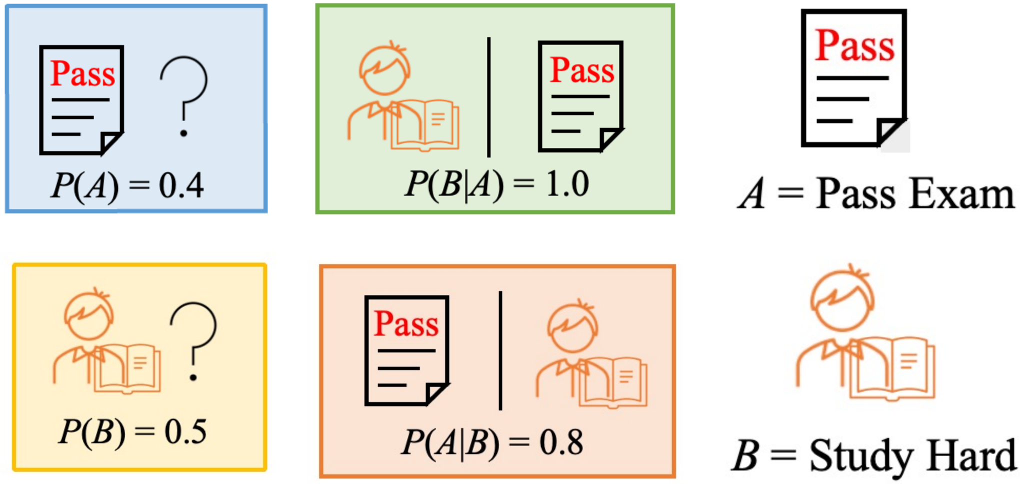

P(A): Prior probability

P(B|A): Likelihood of observing B given A

P(B): Model evidence or marginal likelihood

P(A|B): Posterior probability

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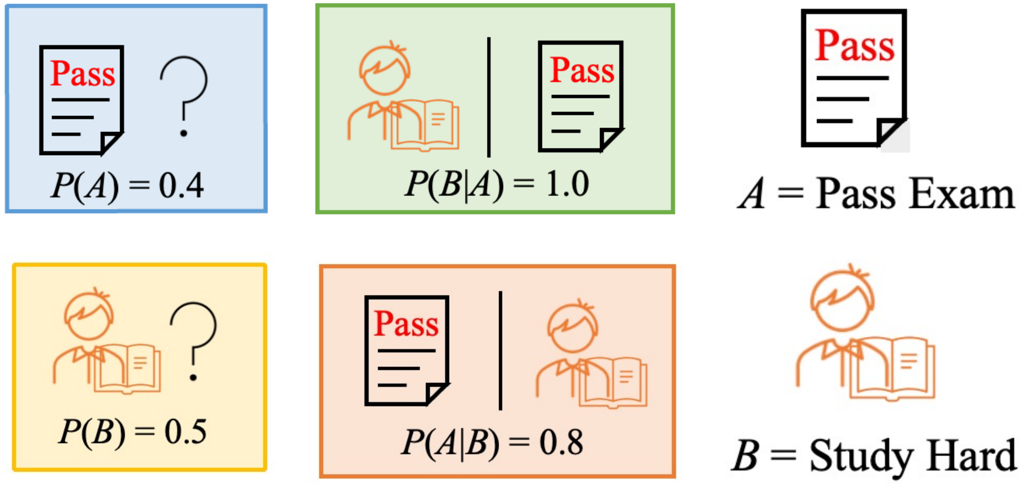

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In essence, Bayes formula says: Posterior $\propto$ Likelihood x Prior

- P(B) is usually not explicitly needed (or sometimes difficult to evaluate)
  - Only P(A) and P(B|A) are needed, as P(A,B)= P(A)P(B|A) and next integration/summation marginalizes 'A' out.
  - If P(A) and P(B|A) are Gaussian, then P(A|B) is Gaussian [1].
  - For arbitrary P(A) and P(B|A), P(A|B) might not have a closed form.

Bayesian Method

Bayesian Method: $P(A|B) = \dfrac{P(B|A)\,P(A)}{P(B)} \propto P(B|A)\,P(A)$

Prior $P(x)$	Likelihood $P(y|x)$	Posterior $P(x|y)$
$\mathcal{N}(x|\mu_0,\sigma_0^2)$	$\mathcal{N}(y|x,\sigma^2)$	$\mathcal{N}(x|\frac{\sigma_0^2}{\sigma^2+\sigma_0^2}y+\frac{\sigma^2}{\sigma^2+\sigma_0^2}\mu,\frac{\sigma_0^2\sigma^2}{\sigma_0^2+\sigma^2})$
$\mathcal{N}(x|\mu_0,\sigma_0^2)$	$\mathcal{N}(y|g(x),\sigma^2)$	No closed form

- For a general case where posterior doesn't have a closed form
  - Variational Inference (e.g., mean-field) uses q_θ to approximate it.
  - Sampling method (e.g., MCMC) is used to draw samples.

Study Case 1: Early- and Late-Stage Performance Estimation

Formulation – Linear regression as an example [11]

Given $D=\{(x_i, y_i) \mid i=1, 2, \ldots, N\}$, find coefficients w such that $\boxed{y \approx \langle w, \phi(x) \rangle}$

Solve the optimization problem: $\min_{\mathbf{w}} \sum_{n=1}^{N} \left(\mathbf{w}^T \phi_n - y_n\right)^2$ linear regression

Least square: $\mathbf{w}_{lr} = \left(\mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{y}$

where $\mathbf{\Phi} \in \mathbb{R}^{N \times F}$ is the sample matrix; n-th row is $\phi_n = \phi(\mathbf{x}_n)$

Question: What if N<F?

Limited data regime, matrix not invertible; Use ridge regression

Study Case 1: Early- and Late-Stage Performance Estimation

Bayesian Approach

Assume prior on model coefficient: $\mathbf{w} \sim p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0, \frac{1}{\alpha}\mathbf{I}\right)$

Likelihood function: $p(\mathcal{D}|\mathbf{w}) = \prod_{n=1}^{N} p(y_n \mid \phi_n, \mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}\left(y_n|\mathbf{w}^T\phi_n, \beta^{-1}\right)$

<=> Assume approximation error $y = \mathbf{w}^T\phi(\mathbf{x}) + \epsilon$ and $\epsilon \sim \mathcal{N}(\epsilon|0, \beta^{-1})$

Posterior has closed form: $p(\mathbf{w}|\mathcal{D}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N),$

where $\mathbf{m}_N = \mathbf{S}_N\left(\alpha\mathbf{m}_0 + \beta\mathbf{\Phi}^T\mathbf{y}\right)$ MAP Estimator

$$\mathbf{S}_N^{-1} = \alpha\mathbf{I} + \beta\mathbf{\Phi}^T\mathbf{\Phi}\ .$$

Study Case 1: Early- and Late-Stage Performance Estimation

MAP Estimator

$$\mathbf{m}_N = \left(\alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \left(\alpha \mathbf{m}_0 + \beta \mathbf{\Phi}^T \mathbf{y}\right)$$
$$= \left(\mathbf{I} + \frac{\beta}{\alpha} \mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{m}_0 + \left(\frac{\alpha}{\beta} \mathbf{I} + \mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{y}$$

How to set m_0, alpha, beta?

Key: Set m_0 with early-stage info!

Step1: Construct a low-fidelity (early-stage) data set

Step2: Perform least square on it to obtain w; take it as m_0

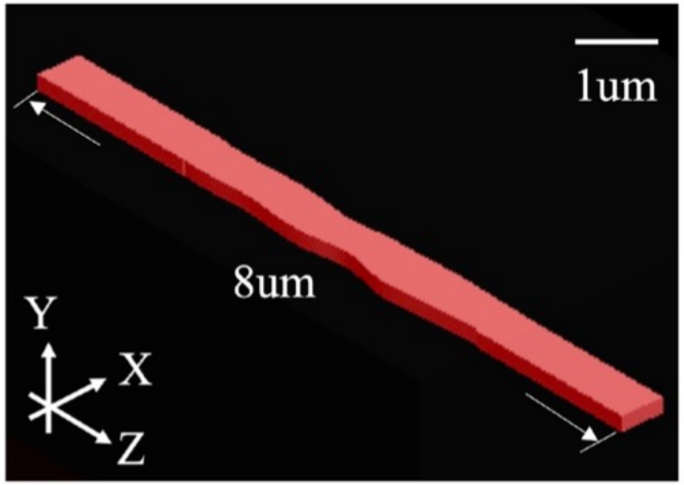
Step3: Combine with only few real data; use the MAP estimator

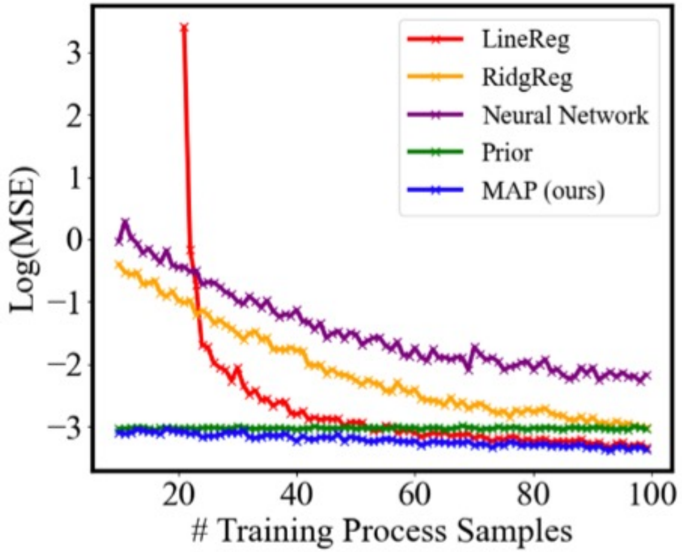
Note: low-fidelity data acquisition is cheap, can be a lot.

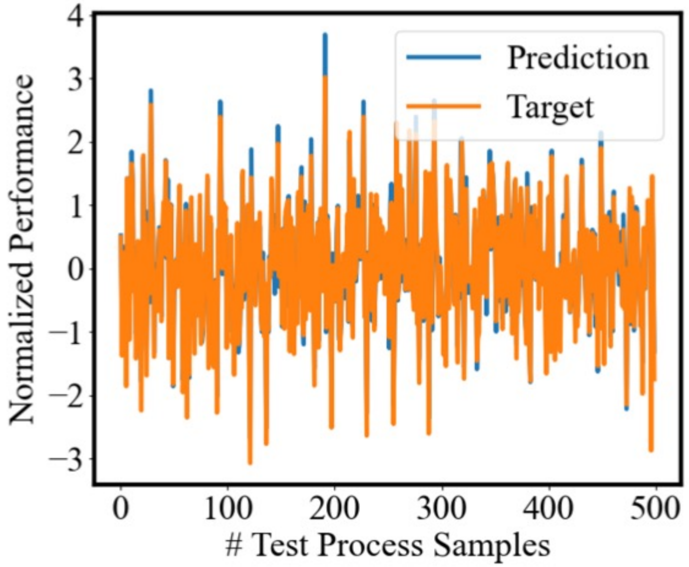
Study Case 1: Early- and Late-Stage Performance Estimation

Numerical Results

Modeling the phase of S parameter under variation





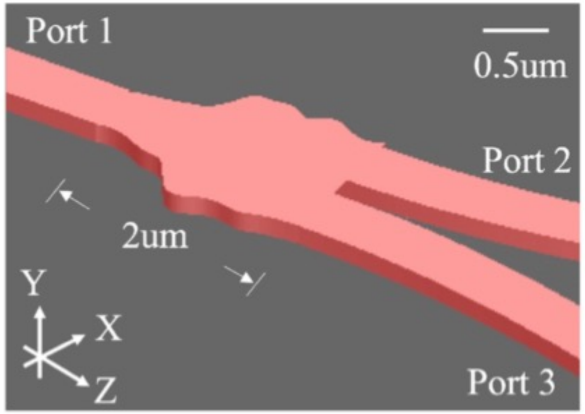


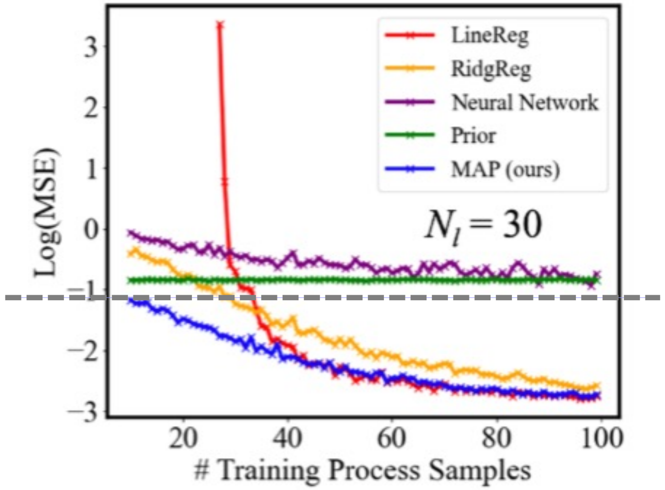
MAP and Prior use 50 low-fidelity samples

Study Case 1: Early- and Late-Stage Performance Estimation

Numerical Results

Modeling the magnitude of S parameter under variation





MAP with N_l = 30 & N= 10

Linear regression with N = 30

Both gives Log(MSE) = -1

Study Case 1: Early- and Late-Stage Performance Estimation

Numerical Results

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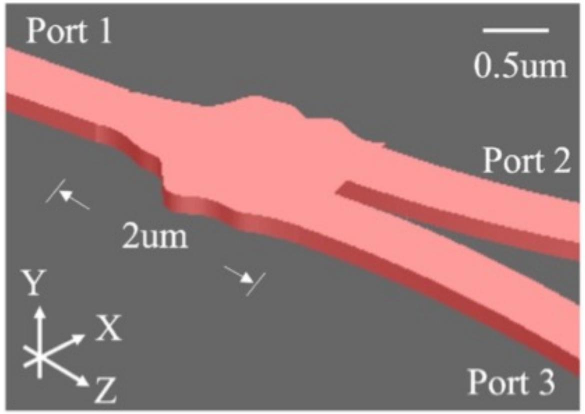
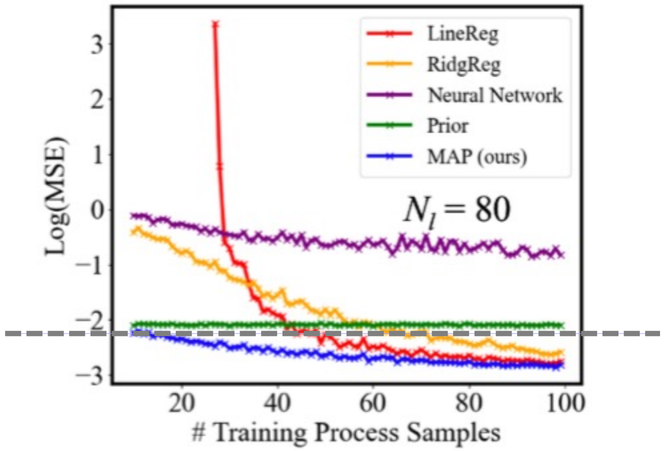




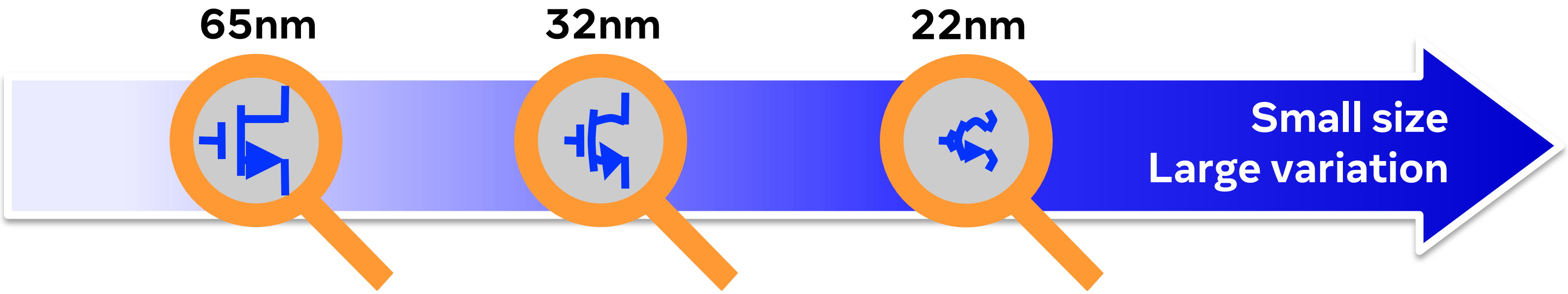
MAP with N_l = 80 & N= 10

Linear regression with N = 40

Both gives Log(MSE) = -2

Remarkable! Only 10 expensive data used in MAP for good accuracy

Study Case 2: Multiple-corner Yield Estimation



Circuit performances uncertainty under process variation

The problem of parametric yield estimation [2]:

Given a desired design, how likely does the fabricated design pass the Spec test?

Math formulation:

The desired design is denoted by **w***.

Process Design Kit (PDK) gives the random variation ε added in manufacturing.

What is the probability that **h=f(w* +** ε**)** locates in a certain “pass” region ?

Study Case 2: Multiple-corner Yield Estimation

Trivial approach --- Monte Carlo

Step 1: Generate N samples $\{\mathbf{w}^* + \varepsilon_1, \mathbf{w}^* + \varepsilon_2, \ldots, \mathbf{w}^* + \varepsilon_N\}$

Step 2: Simulate the corresponding $\{\mathbf{h}_1, \mathbf{h}_2, \ldots, \mathbf{h}_N\}$.

Binary variable
1 = 'inside', 0 = 'outside'

Step 3: Examine each sample locate in Ω or not $\{x_1, x_2, \ldots, x_N\}$

Step 3: Calculate the ratio how many of the N samples locate in Ω: $\beta = \frac{1}{N}\sum_{i=1}^{N} x_n$

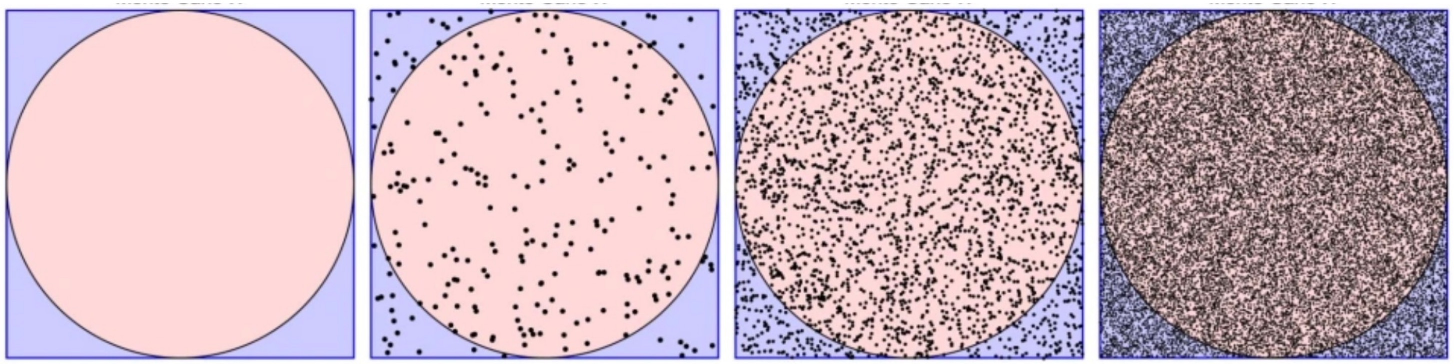


Figure credit: https://shorturl.at/dqsL2

Study Case 2: Multiple-corner Yield Estimation

Reinterpret MC

$$x = \begin{cases} 1 & \text{success} \\ 0 & \text{fail} \end{cases}$$ => $$p(x|\beta) = \begin{cases} \beta & x = 1 \\ 1 - \beta & x = 0 \end{cases}$$ => $$p(x|\beta) = \beta^x (1-\beta)^{1-x}$$

Conditional independence

$$p(D|\beta) = \prod_{n=1}^{N} p(x_n|\beta) = \prod_{n=1}^{N} \beta^{x_n} (1-\beta)^{1-x_n}$$

Maximum Likelihood Estimation (MLE):

$$\max_{\beta} \; p(D|\beta)$$ => $$\beta = \frac{1}{N} \sum_{i=1}^{N} x_n$$

Study Case 2: Multiple-corner Yield Estimation

When multiple corners?

What if we now want to estimate the yield at K corners (e.g., {TT,SS,FF,FS,SF})?

Certainly, we can apply MC independently at each corner: $\beta_k = \frac{1}{N_k} \sum_{n=1}^{N_k} x_{n,k}$

But, if yield at TT is 70%, the yield at other corners should be around 70% as well!

Embed it into the prior distribution!

Study Case 2: Multiple-corner Yield Estimation

Prior distribution: $p(\beta) = \mathcal{N}(\beta|\mu, \Sigma)$

Mu and Sigma are hyper-parameters control the shape of the prior

For example, all K elements in Mu equal 70%, Sigma is an Identity matrix

Likelihood function : $p(D|\beta) = \prod_{n=1}^{N} \prod_{k=1}^{K} \beta_k^{x_{n,k}} (1 - \beta_k)^{1-x_{n,k}}$

Posterior distribution: $p(\beta|D) \propto p(D|\beta)p(\beta)$

Maximum-a-posteriori (MAP) Estimation: $\max_{\beta} \; p(\beta|D)$ How to interpret MAP?

Study Case 2: Multiple-corner Yield Estimation

A few technical details

In essence, the proportional sign means: $p(\beta|D) = \frac{p(D|\beta)p(\beta)}{Z}$

Z is some normalization constant making the expression valid as a distribution

From Bayes theorem Z = p(D) and independent of Beta.

MAP estimation: Maximize the product of the prior and likelihood (Z can be ignored!)

$$\max_{\beta} p(\beta|D) = \min_{\beta} -\ln p(\beta|D) \quad \text{or} \quad \max_{\beta} p(D|\beta)p(\beta) = \min_{\beta} -\ln p(D|\beta) - \ln p(\beta)$$

Equivalently, in logarithm. Advantage: reduce numerical error (Overflow).

Study Case 2: Multiple-corner Yield Estimation

A few technical details

$$\min_{\beta} -\ln p(D|\beta) - \ln p(\beta)$$

where $p(\beta) = \mathcal{N}(\beta|\mu, \Sigma) = \frac{1}{(2\pi)^{K/2}} \frac{1}{|\Sigma|^{1/2}} \exp\{-\frac{1}{2}(\beta-\mu)^T \Sigma^{-1} (\beta-\mu)\}$

$$p(D|\beta) = \prod_{n=1}^{N} \prod_{k=1}^{K} \beta_k^{x_{n,k}} (1-\beta_k)^{1-x_{n,k}}$$

- Observation 1: no closed form for posterior distribution
- Observation 2: Given Mu and Sigma, we can solve the MAP estimator Beta.

How to set hyper-parameters {Mu, Sigma}?

Study Case 2: Multiple-corner Yield Estimation

A simplified algorithm flow; More details refer to [2]

Step1: Given the observation $\{x_{n,k}\}$ and initialize hyper-parameters

All K elements in Mu initialize to the same, and Sigma to a diagonal matrix

Step2: Use IRLS (Newton method) to calculate MAP (i.e., minimize the -log)

An iteration algorithm using gradient and Hessian of the -log

Step3: Use Laplacian approximation to define an approximate posterior

Step4: Use Expectation-Maximization to update hyper-parameters

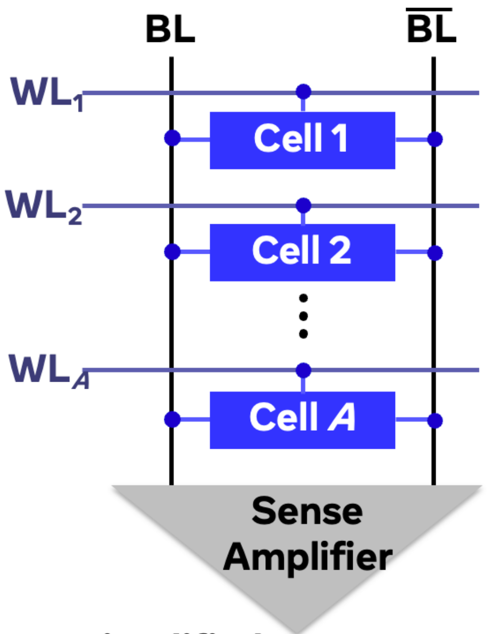
Step5: If convergence not reached, go to Step 2 with the new hyper-parameters

Study Case 2: Multiple-corner Yield Estimation

Numerical examples

Corner	Method	$N = 50$	$N = 100$	$N = 150$	$N = 200$	$N = 250$
TT	MC	4.22	3.15	2.73	2.46	1.75
	BI-BD	3.58	2.88	2.59	2.42	1.73
SS	MC	4.22	3.59	3.18	2.73	2.16
	BI-BD	3.87	3.40	3.08	2.57	2.04
FF	MC	4.73	3.79	3.14	2.28	2.06
	BI-BD	4.51	3.58	2.94	2.04	1.88
FS	MC	7.39	6.01	4.38	3.36	2.57
	BI-BD	5.13	4.09	3.10	2.39	1.85
SF	MC	8.81	6.31	5.86	4.74	3.52
	BI-BD	5.18	4.05	3.88	3.22	2.27

Estimation Error for MC and BI-BD (proposed)



Simplified SRAM array with A cells

Setting: 65nm PDK, five process corners, simulate in Hspice, error from 30 repeated runs

Baseline: independently run MC at each corner (ignore correlations!)

Study Case 2: Multiple-corner Yield Estimation

Some extensions

- Recall we deliberately introduce a Gaussian as prior
  - Not necessarily, this is at our choice.
  - In fact, Gaussian prior + Bernoulli likelihood -> no closed-form posterior
  - How about a prior resulting closed-form posterior? Easier calculation?
  - Indeed, we can do so with the concept of conjugate prior. [3]

Study Case 2: Multiple-corner Yield Estimation

Some extensions

- What if yield is very close to 100%?
  - In literature, usually referred to as rare failure rate estimation [4,5,6,7]
  - Practical usage/example: SRAM cell [4]
  - Challenge: if failure rate = 1e-6, we need (roughly) at least 1e7 MC samples!
  - Problem: Estimate rare failure rate with as few samples as possible
  - Metric: #samples used && logarithm prediction error
  - Past: Multiple-corner failure rate [6]; Recent: single-corner with NF [5]

Where else can Bayes methods be applied?

Minimum Testing [9]

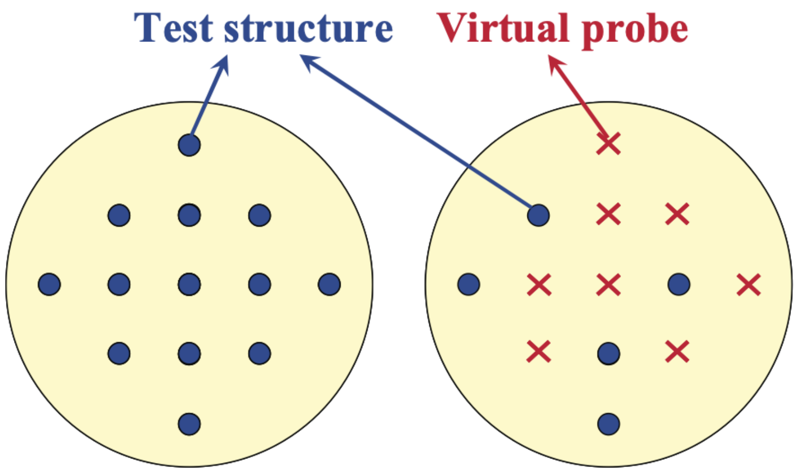


Figure credit: https://shorturl.at/ilGKQ

- Left: Test every location to characterize spatial variation.
- Right: Only few are tested, and others are inferred.
- Prior is introduced to make the system solvable. [?]

Where else can Bayes methods be applied?

Parameter Extraction [10]

- Given limited I-V measurement, extract MOS parameters.
- Prior: Novel transistor relates to existing transistor

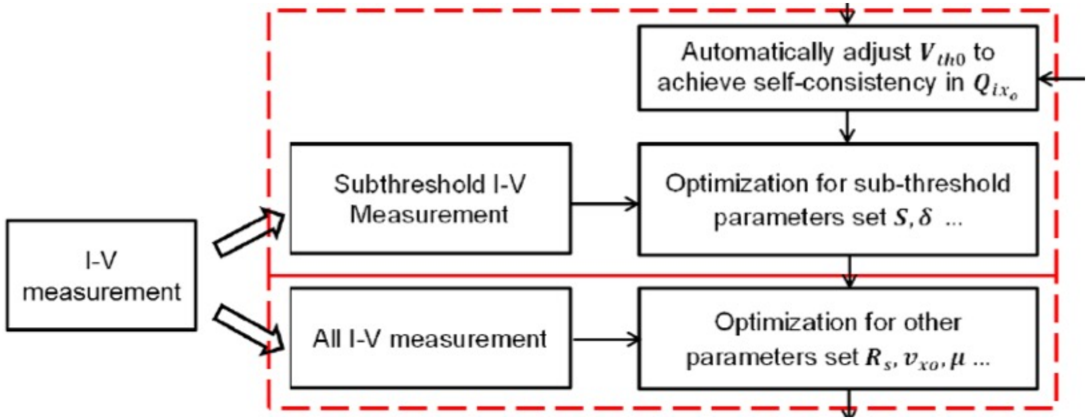
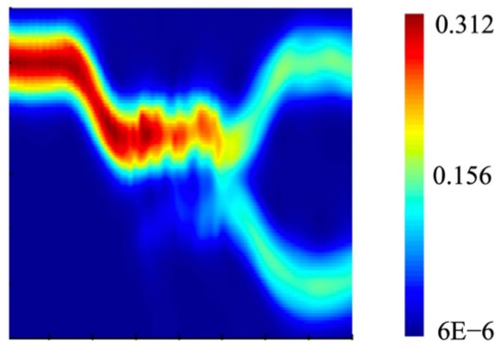


Figure Credit: https://shorturl.at/prNV9

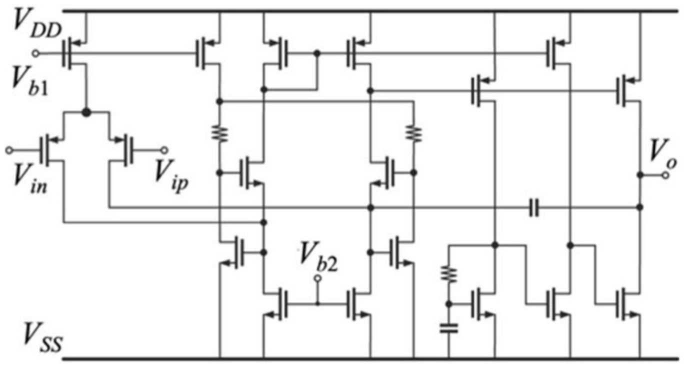
Where else can Bayes methods be applied?

Bayesian Optimization [13,14,15]

- Works with Black-box simulator
- Gaussian process regression (GPR) as surrogate model
- Work well in industrial examples (dim <= 40), e.g., analog sizing, photonic device design.
- Do notice that the definition of GPR requires a mean and a covariance (prior!)



Photonic Y-branch opt



Electronic Opamp

My Recent Focus: Likelihood Free Inference

Classical Parametric MLE: max $p(x|w)$

Where $p(x|w)$ has a parametric form

MAP: Further introduce a prior $p(w)$ and max $p(w|x)$

What is Likelihood Free Inference?

We can only sample an x from $p(x|w)$, but cannot evaluate the distribution value

"simulator-based likelihood"

A lot of approaches, e.g., approximate Bayesian computation (ABC)

Takeaway

- Bayesian methods naturally suit a lot of semiconductor manufacturing problems.
- Need to excavate the knowledge, correlations, and embed them with the prior.
  - Correct embedding improves sample efficiency!
- Usually, the problem is converted to inference a posterior distribution.
  - Posterior might not be analytical --- variational inference, or sampling.
  - EM method for a full Bayesian treatment (inference hyper-parameters)

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