

Rochester Institute of Technology

**RIT Digital Institutional Repository**

---

Theses

---

6-19-2017

## **Bayesian Analysis for Photolithographic Models**

Andrew M. Burbine  
amb7004@rit.edu

Follow this and additional works at: <https://repository.rit.edu/theses>

---

### **Recommended Citation**

Burbine, Andrew M., "Bayesian Analysis for Photolithographic Models" (2017). Thesis. Rochester Institute of Technology. Accessed from

This Thesis is brought to you for free and open access by the RIT Libraries. For more information, please contact [repository@rit.edu](mailto:repository@rit.edu).

# Bayesian Analysis for Photolithographic Models

By

Andrew M. Burbine

A Thesis Submitted

in Partial Fulfillment

of the Requirements for the Degree of

Master of Science

in

Microelectronic Engineering

Approved by:

Prof. \_\_\_\_\_  
Dr. Bruce W. Smith (Thesis Advisor)

Prof. \_\_\_\_\_  
Dr. Robert Pearson (Committee Member & Program Director)

Prof. \_\_\_\_\_  
Dr. Dale Ewbank (Committee Member)

Prof. \_\_\_\_\_  
Dr. Ernest Fokoue (Committee Member)

Dr. John L. Sturtevant (External Collaborator)

Rochester Institute of Technology  
Kate Gleason College of Engineering  
Department of Electrical and Microelectronic Engineering  
June 19<sup>th</sup>, 2017

## Abstract

The use of optical proximity correction (OPC) as a resolution enhancement technique (RET) in microelectronic photolithographic manufacturing demands increasingly accurate models of the systems in use. Model building and inference techniques in the data science community have seen great strides in the past two decades in the field of Bayesian statistics. This work aims to demonstrate the predictive power of using Bayesian analysis as a method for parameter selection in lithographic models by probabilistically considering the uncertainty in physical model parameters and the wafer data used to calibrate them. We will consider the error between simulated and measured critical dimensions (CDs) as Student's  $t$ -distributed random variables which will inform our likelihood function, via sums of log-probabilities, to maximize Bayes' rule and generate posterior distributions for each parameter. Through the use of a Markov chain Monte Carlo (MCMC) algorithm, the model's parameter space is explored to find the most credible parameter values. We use an affine invariant ensemble sampler (AIES) which instantiates many *walkers* which semi-independently explore the space in parallel, which lets us exploit the slow model evaluation time. Posterior predictive checks are used to analyze the quality of the models that use parameter values from their highest density intervals (HDIs). Finally, we explore the concept of model hierarchy, which is a flexible method of adding hyperparameters to the Bayesian model structure.

# Table of Contents

Abstract .....	2
List of Figures .....	5
Introduction and Motivation .....	10
Chapter 1 – Photolithographic Systems .....	13
Chapter 2 – Statistical Modeling.....	19
Probability Distributions .....	19
Uncertainties as Distributions .....	22
Linear Regression.....	26
Chapter 3 – Bayesian Analysis .....	30
Bayes’ Theorem .....	30
Markov chain Monte Carlo algorithms .....	31
The Linear Model example, revisited .....	33
The Likelihood Function.....	35
Implementation in Python .....	37
Chapter 4 – Results and Analysis.....	41
Initial, exploratory run .....	41
Adding n & k of the resist and ARC .....	46
Hierarchy in the Model .....	50
The influence of prior distribution choice.....	54

Posterior predictive checking and comparison to incumbent process .....	58
Conclusions .....	60
References .....	61

## List of Figures

Figure 1: An example of using optical proximity correction to increase the image fidelity during pattern transfer .....	11
Figure 2: There's been a large increase on published papers on Bayesian inference and analysis methods. ....	13
Figure 3: Schematic of a Köhler illumination system used for photolithographic processing. The pattern on the mask is minified by 4x and transferred to the wafer, where its latent image indicates where the deprotection reactions in the photoresist will result in removal during development.....	14
Figure 4: Various illustrations of image fidelity as $k_1$ and the minimum feature size decrease for a 193nm non-immersion system at 0.85 NA. At $k_1 = 0.3$ , the feature no longer resolves a usable resist contour. However, through various techniques described in the figure, imaging is still possible. [7].....	16
Figure 5: Screenshot from Calibre WORKbench showing the simulated contour (red) of a photomask (white) and a gauge (vertical line) which measures the CD at this location. .	17
Figure 6: Histogram of 1000 points generated from a normal distribution with mean 0 and standard deviation 2. In red is the exact probability density function for the distribution.	21
Figure 7: Illustration from Sir Francis Galton of "the bean machine" which physically demonstrates the central limit theorem. ....	21
Figure 8: Student's t-distribution with various values for $\nu$ , showing the change in the tails of the distribution. As $\nu$ approaches infinity, the Student's t-distribution becomes the normal distribution. ....	26

Figure 9: Sample 2D data generated with error bars representing measurement uncertainty. The line represents the function used to generate the sample points. This data will be used in subsequent examples of linear modeling;  $m_{\text{true}} = -0.9594$ ,  $b_{\text{true}} = 4.294$  and  $f_{\text{true}} = 0.534$  (where  $f * y * U(0, 1)$ )..... 27

Figure 10: Sample data and the model generated by least squares regression. Parameter estimates are  $m_{\text{ls}} = -1.104 \pm 0.016$  and  $b_{\text{ls}} = 5.441 \pm 0.091$  ..... 28

Figure 11: Sample data with the maximum likelihood model solution, in magenta. Parameter estimates are  $m_{\text{mle}} = -1.003$ ,  $b_{\text{mle}} = 4.528$  and  $f_{\text{mle}} = 0.454$ ..... 29

Figure 12: Figure with caption from Goodman and Weare's publication showing a stretch move [17] ..... 32

Figure 13: Posterior distribution for the parameters in the linear model. Top plots are 1D histograms, others are bivariate density plots. True values are shown in blue lines..... 34

Figure 14: Red shows the true model. The rest of the lines are samples form the posterior distribution showing various candidate models. Bayesian analysis sees the solutions as a probabalistic entity. .... 34

Figure 15: Flow diagram describing the goal of Bayesian analysis for photolithographic modeling. The model, which has fixed and free parameters, describe the photolithographic manufacturing process and produce simulated contours of the resist based on the mask layout. These are ideally as close as possible to the CD measurements from the wafer fab, which are shown to be drawn from a distribution due to stochastic effects. .... 37

Figure 16: Flow diagram for generating the posterior distribution..... 39

Figure 17: The seven dimensional posterior distribution using 100 gauges during the posterior maximization with AIES..... 42

Figure 18: 2nd calibration from an independent random sample of 100 gauges from the master set. ....	44
Figure 19: 3rd calibration from an independent random sample of 100 gauges from the master set .....	45
Figure 20: The full 11 dimensional posterior space. Blue lines indicate values given with the testcase for each parameter. Thus, differences between the given and posterior indicate the benefit from optimizing these parameters.....	47
Figure 21: Magnified plot of the resist and ARC n & k posteriors.....	49
Figure 22: Graphical representation of the simple one level model hierarchy used so far.	50
Figure 23: Graphical representation of two level model hierarchy using feature types to group the gauges.....	51
Figure 24: The posterior distribution triangle plot for the two-level hierarchical model and n & k film stack parameters. ....	52
Figure 25: The posterior distribution triangle plot for the simple two-level hierarchical model. ....	53
Figure 26: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a uniform prior. [24] .....	54
Figure 27: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a normal prior close to the likelihood. [24] .....	55
Figure 28: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a prior far from the likelihood. [24].....	56
Figure 29: Posterior distributions for two optimizations on just mask parameters comparing the use of normally distributed priors to uniformly distributed priors.....	57





## List of Tables

Table 1: Parameters in the model along with their associated prior distributions and absolute limits. Beamfocus and metrology plane are relative to the top of the resist stack, such that 0 = top, and positive is into the plane of the wafer. ....	38
Table 2: The film stack properties added to the parameter space along with their priors and truncated limits.....	46
Table 3: Comparison of nm RMS error between simulated models and wafer data for basic and complex models generated with different random samples of gauges. Compare to incumbent RMS minimization of 4.11.....	58

## Introduction and Motivation

The pace of microelectronics manufacturing capability is dictated each year by the International Technology Roadmap for Semiconductors (ITRS) [1] with goals centered on scaling devices smaller and smaller and addressing associated challenges, such as mitigating line edge roughness and increasing critical dimension (CD) uniformity across a wafer. Historically, these challenges rested on the shoulders of lithographers and the chemists who created the photoresists necessary for patterning. Today, the challenges are also felt by the layout designers, who must seek regularity in their designs and plan for such things as multiple patterning, and the tool manufacturers who must integrate increased metrology and uniformity controls on intra- and inter-wafer effects.

The goal of solving these challenges is to increase the processing power and memory capabilities for the ever expanding usage of electronics, which enable new technologies and a higher quality of life. Amusingly, one of the key uses for increased processing power and memory capabilities is in the lithographic field itself – the modern lithographer operates at the limits of his or her lithographic scanning tool and must make use of many resolution enhancement techniques (RET), chief among them, optical proximity correction (OPC), an example of which can be seen in Figure 1. Accurate OPC models require powerful computers to operate on a full-chip layout due to the immense number of patterns [2].

OPC compensates for image errors due to operating at or near the diffraction-limited resolutions of the scanners used to transfer the design intent image to the wafer. A measure of a system's resolution is typically given by Rayleigh's criterion, seen in Equation 1, where the smallest critical feature width, or minimum half pitch, is determined by the wavelength  $\lambda$ , the numerical aperture NA and the  $k_1$  factor [3].

$$halfpitch_{min} = \frac{k_1 \lambda}{NA} \quad (1)$$

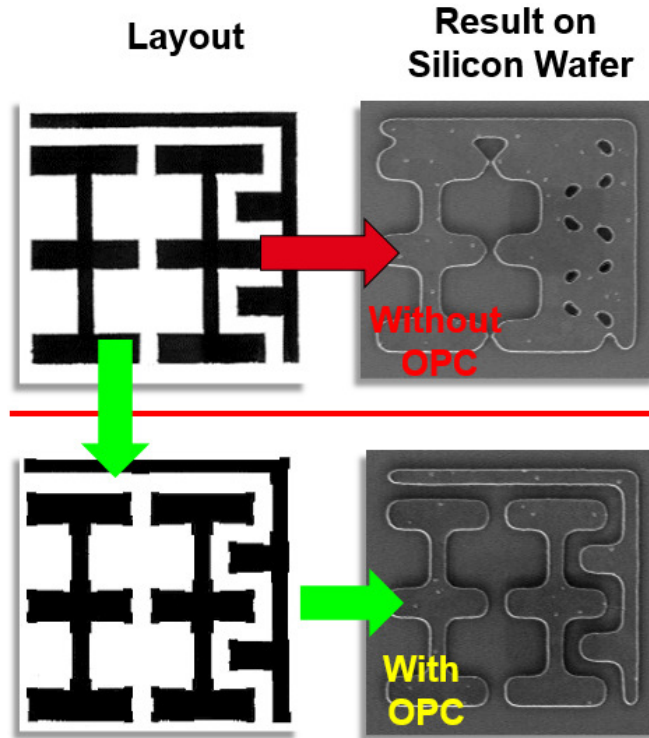


Figure 1: An example of using optical proximity correction to increase the image fidelity during pattern transfer

Thus, for a modern 193 nm immersion system, operating at an NA of 1.35 and a  $k_1$  factor of 0.3, a minimum half pitch of about 42 nm is achievable. OPC is a key method for reducing the usable  $k_1$  factor of a manufacturing process, decreasing the minimum pitch and keeping pace with the ITRS roadmap.

In order to apply OPC to a full-chip layout, fast models are needed to simulate resist contours from layout geometries. Model-based OPC methods simulate the changes to the layout and seek to find solutions to make dense patterns resolve with robustness to small changes in dose and focus (the so called process window). These models make use of physically based parameters from the system, such as film stack properties like the  $n$  and  $k$  of various materials in models of the photomask which effect the transmission and phase of the light used for exposure. Other parameters include: film stack properties in the wafer stack (photoresist, anti-

reflective coatings, under-layers and the substrate itself), the wavelength of light used in exposure and a Jones pupil of the optics of the scanner and any pellicle (protective film over the photomask) [4].

These parameters are tuned in a model training exercise by matching simulated CD measurements to measurements taken from a wafer. Thousands of CDs are collected by a CD scanning electron microscope (CDSEM) which produce images similar to the right side of Figure 1. Current day practice involves minimizing the root mean square error of the measured CDs to the simulated CDs via gradient-descent like optimization methods.

Unfortunately, this ignores a key aspect of the model building process: uncertainty. Measurements taken from a CDSEM are not always accurate due to the low resolution of the SEM and the difficulty in resolving the edge of a sloped photoresist sidewall profile from a top-down image. Additionally, there are uncertainties in some of the parameters which are fixed in the models, such as the thickness of the photoresist or its optical constants (refractive index  $n$  and extinction coefficient  $k$ ). Though in the past these uncertainties may have been well beyond the scope of critical sources of error in the modeling process, today's OPC demands accuracy to the single digit nanometer or below level.

Additionally, modelers may often have reasons to believe parameters are more likely to have accurate solutions at certain values over others. For example, the mask absorber sidewall angle is often *expected* to be at 86 degrees, plus or minus a degree, rather than at, for example, 90 degrees. Modelers may also have expectations on the amount of variance possible for a parameter, for example the photoresist thickness might vary by 1-2 nm but not more.

Under a Bayesian framework these uncertainties and a priori knowledge can be incorporated into the model building process directly, as we consider each parameter to come

from a distribution of possible values. Additionally, CDSEM measurements are often taken from several dies or wafers and have the number of images used to produce the single average value reported, as well as the standard deviation of those measurements. This information can be directly incorporated into the cost function that drives the optimization procedure.

The goal of this work is to apply Bayesian analytic methods to produce photolithographic models that better utilize available information and incorporate the uncertainties that exist in both the model parameters and the measurements that are used to inform those parameters. Bayesian methods have seen an increase in usage (Figure 2) and maturity as increased computational power has enabled stronger algorithms needed to converge to solutions for high-dimensional parameter spaces.

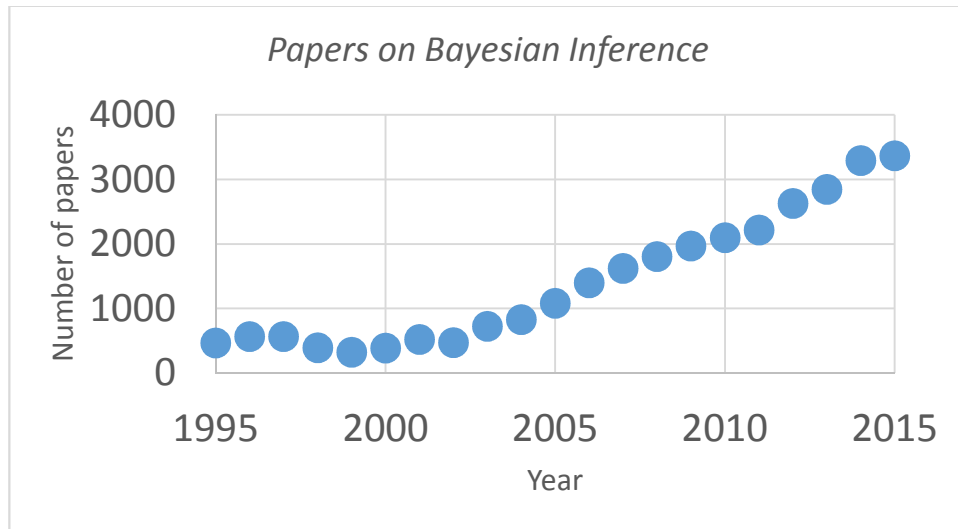
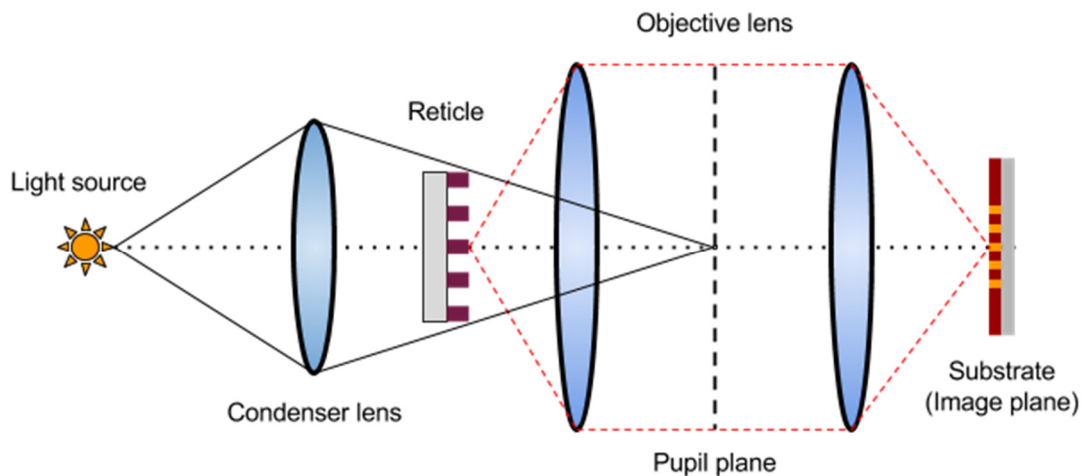


Figure 2: There's been a large increase on published papers on Bayesian inference and analysis methods.

## Chapter 1 – Photolithographic Systems

Photolithography is the process by which a pattern is transferred from a mask, or reticle, to a wafer using light and a photosensitive thin film (photoresist). After the wafer is exposed to DUV (or EUV) light, in a positive-tone resist, those areas can be dissolved away with a developer solution, typically a strong base. This then enables either etching into the material

below the photoresist or deposition of a new material in the resulting voids. Thus, lithography is at the center of constructing microelectronic devices: repeated deposition and etching steps are done in specific patterns created by a series of exposures for different layers of the device. These layers form and provide connections between transistors, which are arranged to create logic gates that are used for computation, memory storage or other functions.



*Figure 3: Schematic of a Köhler illumination system used for photolithographic processing. The pattern on the mask is minified by 4x and transferred to the wafer, where its latent image indicates where the deprotection reactions in the photoresist will result in removal during development*

Since smaller and smaller feature sizes enable more computing power per area of a chip, we must consider what defines an optical system's capability. Equation 1 defines the minimum halfpitch by what is known as Rayleigh's criterion. From this equation two things are immediately apparent: increasing the lens size, NA, and reducing the wavelength,  $\lambda$ , will reduce the feature size. For several decades, these were the main strategies for continued scaling in the industry, which moved swiftly from 365 nm to 248 nm and finally (for transmissive optics) 193 nm. Tools are currently in evaluation and technology research and development at 13.5 nm (EUV, reflective optics) after almost a decade since 193i was introduced for use in production manufacturing. 193 nm immersion systems increased the NA of these systems beyond 1.0

through the use of water between the lens and substrate [5]. Research was done exploring 157 nm as a successor to 193 nm, but ultimately did not occur due to a myriad of challenges [6].

The other parameter in the equation,  $k_1$ , is known as a ‘process factor’ which encapsulates many other performance criterion in the system, such as photoresist resolution (the ability of the photoresist to threshold the image with minimal loss), mask properties (such as a thin absorber to limit 3D mask effects) and illumination properties (see below).  $k_1$  can be seen as a compromise between image degradation and the photoresist’s robust ability to capture low-intensity modulation to form binary images.

Figure 4 illustrates how  $k_1$  for a non-immersion (0.85 NA) 193 nm system relates to image fidelity and various so-called resolution enhancement techniques (RET) used to undo its effect on imaging. When  $k_1$  is high, imaging is easily achieved by the system and as it decreases with the minimum desired feature size, eventually the image fidelity drops below a tenable level. Off-axis imaging (OAI) refers to the use of partially incoherent sources. Initial OAI technologies employed various primitives, such as dipoles and quasars, to improve imaging. Today, sources can be pixelized and are produced through source-mask optimization (SMO) as a first step during technology development.



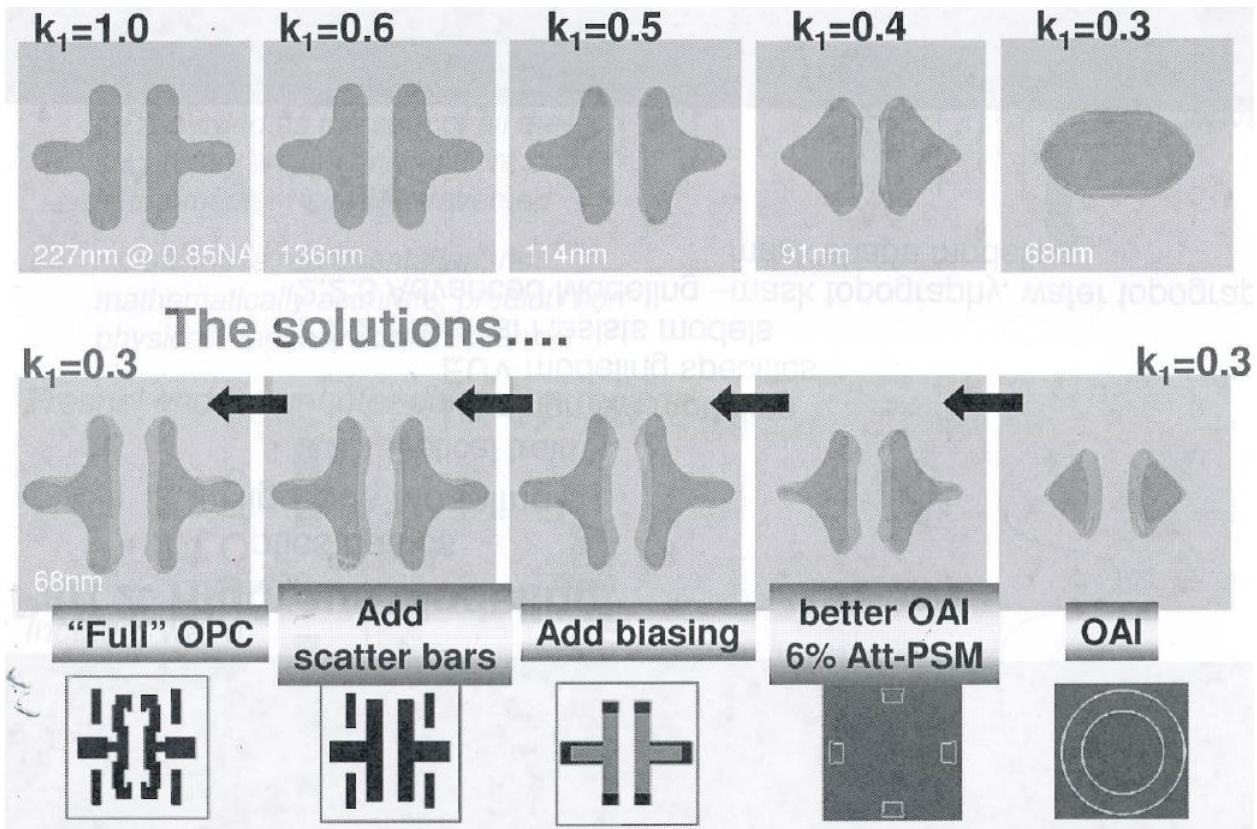
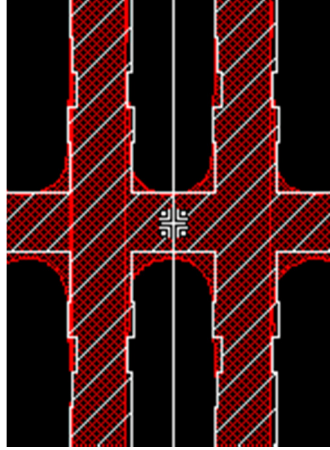


Figure 4: Various illustrations of image fidelity as  $k_1$  and the minimum feature size decrease for a 193nm non-immersion system at 0.85 NA. At  $k_1 = 0.3$ , the feature no longer resolves a usable resist contour. However, through various techniques described in the figure, imaging is still possible. [7]

Finally, a key technology for enabling low- $k_1$  imaging and increasing the resolution of photolithographic systems is optical proximity correction (OPC), shown in the figure as the ultimate solution for producing usable images for a given process condition. Figure 5 shows the simulation output using a photolithographic model in Calibre WORKbench. During iterations of OPC, edges of feature polygons are moved with the goal of minimizing the edge placement error (EPE) between the simulated resist contours and the target shape.



*Figure 5: Screenshot from Calibre WORKbench showing the simulated contour (red) of a photomask (white) and a gauge (vertical line) which measures the CD at this location.*

Early OPC techniques were rule-based – edges were moved based on a rule deck to do such things as compensate line-end pullback by adding hammerhead shapes to tip-to-tip features or biasing the edge of an array with smaller features to compensate for edge effects. Rule-based techniques were fast and could be performed on an entire chip to improve imaging performance. However, eventually, special algorithms were developed to be able to perform simulations of aerial images fast enough to be usable on a full chip [8], [9], [10]. Additionally, computing power advanced enough to enable such simulations, which is to say that advancing lithographic techniques enabled the ability to further advance lithographic techniques.

Thus, model-based OPC was born and a new branch of enabling technologies and methodologies came along with it. These methods include: sum of coherent systems decomposition (SOCS), domain decomposition methods (DDM), hybrid Hopkins-Abbe method for source sectorization (HHA) and resist compact models (CM1) [11], [12], [13], [14]. Each enabled more accurate simulation of the final resist or etch contour on the wafer level from simulations of the photomask through the imaging system. Typically, models are calibrated to wafer CD measurements on a test mask, which contains large arrays of various feature types with variations through feature and pitch dimensions. Then, when it is time to

perform OPC, these models are used to modify the full chip geometries to match the design intent (or target layer) within some tolerances, usually through focus to mitigate errors caused by wafer topography.

The subject of this thesis is to improve the accuracy of the models used by finding more accurate representations of the physical parameters in the model. To do this, we consider the parameters as coming from unknown distributions and the CDs collected of the wafer as having uncertainty derived from being drawn from a distribution, based on the standard deviation of those measurements. These distributions are represented in a Bayesian framework, which will be explained in further detail.

## Chapter 2 – Statistical Modeling

### Probability Distributions

In the field of data science, models are created to describe data sets which can be used to make predictions, gain insight on the system that produced the data set, or characterize the stochastic elements of the system. Statistical modeling differs from mathematical modeling in that part or parts of the model are non-deterministic; some variables in the model do not have specific values but instead are drawn from probability distributions.

A probability distribution is a mathematical definition of a function that satisfies several properties: 1) evaluates to a non-negative number for all real inputs, 2) the sum (or integral) for all possible inputs is 1, and 3) the probability of a specific value (or a value between bounds) is the result of the evaluation of the function.

The simplest and most classic example of a probability distribution is the Bernoulli distribution, which describes a system in which the outcome is either 0 or 1. We can define the probability of the outcome 1 as  $\Pr(X = 1)$ , which is equal to  $1 - \Pr(X = 0)$  to be equal to  $p$ . A so called “fair” coin, for example, would be described by a Bernoulli distribution with  $p = 0.5$ , because the coin is equally likely (50%) to produce ‘heads’ (an outcome of 1) as it is ‘tails’ (an outcome of 0). Defined more rigorously, the probability mass function for the Bernoulli distribution over possible outcomes  $k$  is defined as

$$f(k; p) = p^k(1 - p)^{1-k} \quad (2)$$

Thus, a *model* that describes the process of flipping a coin would be the random variable  $B$ , which represents the Bernoulli distribution with parameter  $p$ , describing the probability of heads for that coin. The value of  $p$  could be known, assumed, or desired to be found – each scenario represents a different use for the model of the coin. For physical coins, we would

typically either assume a value or seek to find it. If we were simulating a coin, we would be able to set it, by *defining* its value to produce a random variable that has the properties we desire.

Note that by applying a Bernoulli distribution to any real world scenario, we have already made assumptions about the nature of the system. For example, a real world coin has some chance, although very small, of its end state after a flip *not* being heads or tails – it could end up wedged between floorboards upright on its edge, or roll into a sewer grate where we cannot observe it. However, by using the Bernoulli distribution, which only has outcomes of 1 or 0, we do not account for other scenarios in the model, thus we have defined a *scope* for what we wish to predict or measure.

The Bernoulli distribution is a discrete, univariate probability distribution, meaning that its outcomes are singular in dimension and from a finite set, defined by a probability *mass* function. Conversely, a univariate continuous distribution is defined by a probability *density* function and has infinite possible outcomes. Perhaps the most common example is the normal (or Gaussian) distribution, which has the probability density function defined in Equation 3.

$$f(x | \mu, \sigma^2) = \frac{1}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (3)$$

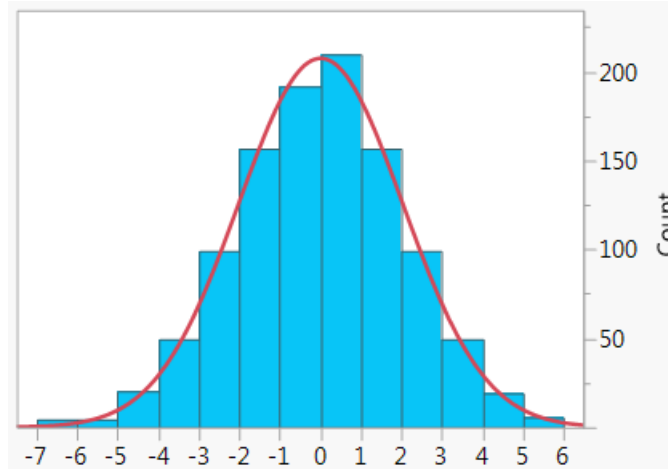


Figure 6: Histogram of 1000 points generated from a normal distribution with mean 0 and standard deviation 2. In red is the exact probability density function for the distribution.

The normal distribution is particularly useful because of the central limit theorem, which states that the arithmetic mean of a set of many independent and identically distributed (i.i.d.) will be approximately normally distributed, regardless of the underlying distribution of the constituents of the set. Figure 7 shows an illustration by Sir Francis Galton of *the bean machine* which is designed to demonstrate the central limit theorem.

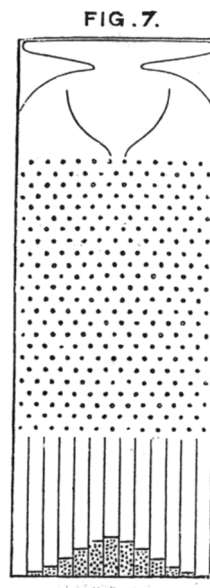


Figure 7: Illustration from Sir Francis Galton of "the bean machine" which physically demonstrates the central limit theorem.

The machine is set up to have balls dropped at the top and bounce on the pins as they descend toward the bins at the bottom of the machine. For each pin, the balls have a probability of going to the left of the pin or the right of the pin as they descend due to gravity. That can be represented as a Bernoulli probability, perhaps with  $p = 0.5$  for equal chance of left or right. However, the result of these probabilities in the end tends toward a normal distribution of ball positions, as shown in the illustration.

For data scientists, this means that we can make assumptions about the data we collect and measure when studying a system. In the general case, many data points are generated under ideally identical circumstances, meaning that each one is drawn from a distribution of possible values when all but one source of variation is eliminated. That is, if one were to measure the heights of 100 individuals from a random sampling of the population, they are expected to approximate a normal distribution, because of the central limit theorem.

Because probability distributions are defined mathematically, many interesting properties can be derived directly, such as the expected value (also known as the mean), which is the weighted average of the possible values produced by the distribution, and the variance, which is a measure of the dispersion of the distribution. For the normal distribution, the parameters conveniently define its mean, location parameter  $\mu$ , and variance, scale parameter  $\sigma^2$ . After observing some  $n$  measurements, we can *estimate* the distribution parameters of the population that best create the samples we observed, which let us make inferences about future observations.

## Uncertainties as Distributions

OPC models can describe the entire patterning process including optics, resist, and etch, in a single lumped representation, or can be discretized to characterize each module. While

details vary depending upon the exact software being used for OPC, there are several different classes of parameters associated with the calibration of the mask, optical, resist and etch process models. There are parameters which are directly measurable or known as designed values, and are primarily associated with the mask and optical systems. Mask parameters include global edge bias, 2D corner rounding, 3D geometry details and optical properties of the film stack. Optics parameters include, for example, wavelength, numerical aperture (NA), illumination intensity profile, and film stack thicknesses & optical constants. While all of these values may be input to the model as is, to the extent that their accuracy is not perfect they can also be adjusted over a small range during the optimization. Care must be taken, however, in allowing these parameters to move too far from their design values, as this may result in a less physical model.

A second class of parameters are those associated with physical phenomena, where direct measurement is not done, but rather the model contains mathematical proxies for the parameter, but usually without a direct mapping correlation. These are the parameters which are most often associated with the complex photoresist PEB, develop, and etch chemical kinetics. A final class of calibration options includes software knobs for altering the approximations used in the model, such as number of optical kernels, or optical diameter, and resist or etch model form.

In order to quantify the uncertainties we have in the parameters in the model, we can use a probability distribution. For example, we may be informed that the resist film thickness is 86 nm – with no other information, we are left to our own devices about an assumption to make about its uncertainty. However, given that this came from a measurement (or measurements) we can assume, thanks to the central limit theorem, that resist thicknesses for



wafers in the fab likely follow a normal distribution, and are free to choose some small variance, perhaps  $\sigma^2 = 1$  nm.

It is this author's experience that, for many of the measurements necessary to complete lithographic modeling, variance information is left out when reporting the values of known physical parameters. However, by stating ones assumption, we open the area for discussion for those with expertise to add what they know about the system. By being explicit, the assumptions that go into the model can be discussed, where normally the assumptions would go undefined. For example, one may now be motivated to check the historical data on resist measurements, and report a *real* estimate of their probability distribution backed up by observations in the fab, which would improve the quality of the model generation process.

Each parameter in our model should receive this treatment to best understand how each part of the system may be varying. Statistical process control engineers collect some of this data, but other parts of the model are left unobserved or rarely observed, but we must still come to a consensus on how we define the variance for each parameter in the model, because in manufacturing there are always tolerances and stochastic effects that alter the intended values for every piece of the process. Luckily, because the efforts of manufacturing are successful, we know that they have small enough variances to let these non-idealities become absorbed, however it is best to understand thoroughly these tolerances and incorporate them into our models of the system.

Finally, the goal of the model is to predict critical dimensions (CDs) that were measured by a scanning electron microscope (SEM) after the to-be-modeled layer was exposed in the fab. These measurements also have uncertainties, as they are measured across multiple dies on a wafer and multiple wafers in a lot. For the purposes of OPC, which can only generate a single

mask for production, we must accept the variability as part of the process, and seek to consider the true and unknown values of these measurements as probability distributions.

Luckily, for most data collection routines, while the average CD across a wafer or wafers is reported, we typically also receive the number of measurements that were done as well as their standard deviation. We can use this information *directly* to inform the probability distributions we wish to use in our models.

One difficulty when calibrating models for OPC is the need for a staged approach. Typically, optics and mask parameters are calibrated (together or sequentially), and then the resist is characterized (afterwards, an etch model can also be applied, though the most of the effort centers around achieving a good resist model). Because there is no resist model present when calibrating the optics and mask parameters, and it is not common to have aerial image measurements during this step, aerial image CDs are calibrated to on-wafer resist CDs.

For this reason, the non-standardized Student's  $t$ -distribution is used over the normal distribution to consider the CD measurements' uncertainty. Typically, the Student's  $t$ -distribution is employed when estimating the mean of a normally distributed population when the sample size is small and the population standard deviation is unknown. The non-standardized Student's  $t$ -distribution has three parameters: the mean,  $\mu$ , the degrees of freedom,  $\nu$ , and the scale parameter  $\sigma$ , which should not be confused with the standard deviation. As  $\nu$  (the number of samples) approaches infinity, the Student's  $t$ -distribution becomes the normal distribution.

$$p(x | \nu, \mu, \sigma) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\pi\nu\sigma}} \left( 1 + \frac{1}{\nu} \left( \frac{x - \mu}{\sigma} \right)^2 \right)^{-\frac{\nu+1}{2}} \quad (4)$$

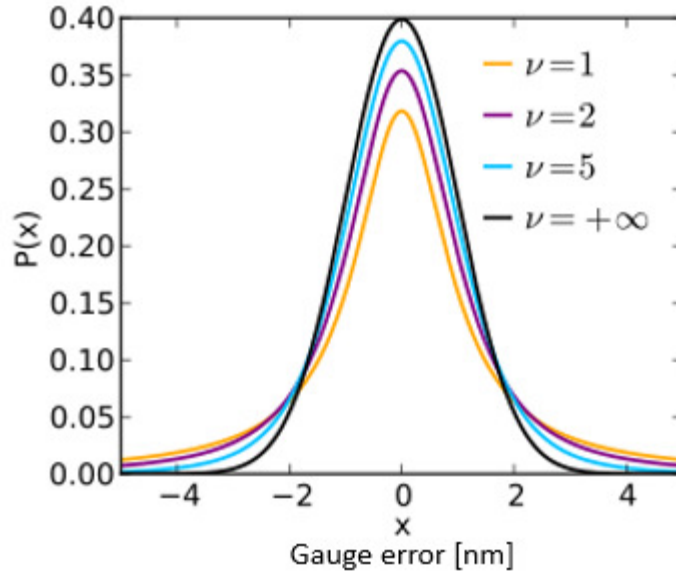


Figure 8: Student's  $t$ -distribution with various values for  $\nu$ , showing the change in the tails of the distribution. As  $\nu$  approaches infinity, the Student's  $t$ -distribution becomes the normal distribution.

The larger *tails* of the Student's  $t$  give credibility to values further from the mean, which is desirable given the aerial-to-resist calibration, allowing the error of the simulated CD to leave room for the resist model to fill in later. That is, we expect error in the model when we leave out resist effects, and we do this by using the Student's  $t$  over the normal distribution.

### Linear Regression

We can use variables to create relationships by casting them into the rolls of *predictor* and *predicted*. Traditionally, this comes in the form of a predictor  $x$  and predicted  $y$ , which can also be called the independent  $x$  and dependent  $y$ . Under the simple linear regression model, we allow the predicted variable to take on probabilistic residual noise, typically normally distributed.

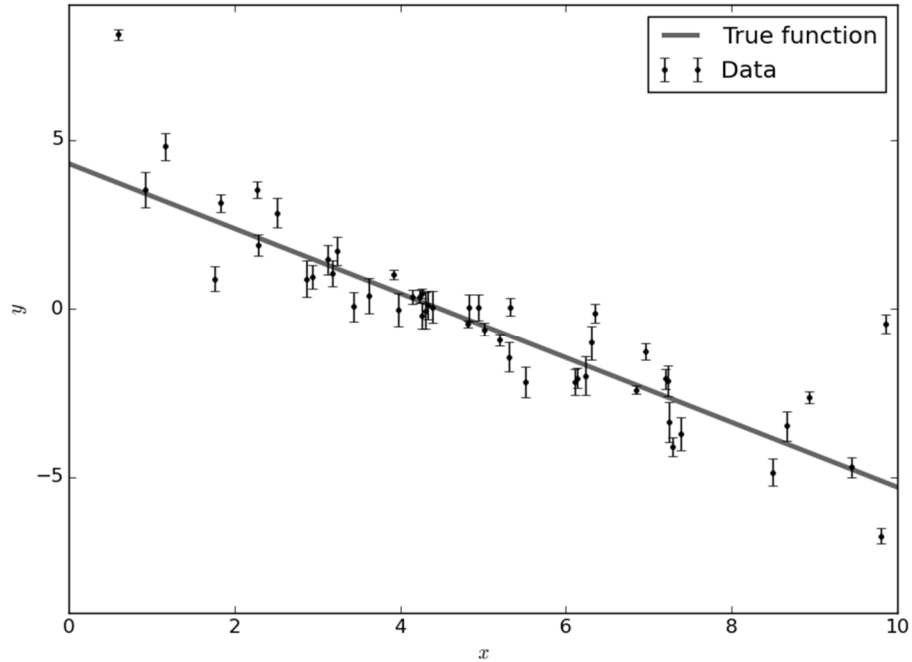


Figure 9: Sample 2D data generated with error bars representing measurement uncertainty. The line represents the function used to generate the sample points. This data will be used in subsequent examples of linear modeling;  $m_{\text{true}} = -0.9594$ ,  $b_{\text{true}} = 4.294$  and  $f_{\text{true}} = 0.534$  (where  $f \sim y \cdot U(0, 1)$ ).

If, while taking measurements from samples, we observed two variables from each, an  $x$  and a  $y$  value, and wanted to quantify a relationship between these, one of the most basic methods would be to employ what is known as a generalized linear model. In the general case, we would call the  $y$  our dependent variable and  $x$  the explanatory variable. We would seek to find the relationship such that

$$\mathbf{y} = \mathbf{mx} + \mathbf{b} + \boldsymbol{\epsilon} \quad (5)$$

and for each observation we would have:

$$y_i = m_i x_{ip} + b_i + \epsilon_i \quad (6)$$

Figure 9 shows sample data generated from an underlying function which is the true generating function for the data. Any models we employ will seek to match the parameters of this generating function, shown in the caption of the figure. For some models, we can even

estimate the parameter  $f$  which models the uncertainty in the measurements drawn from a uniform random variable.

One such solution for estimating the parameters is linear least squares regression. For each observation, we assume normally distributed errors. Figure 10 shows the results of such a regression.

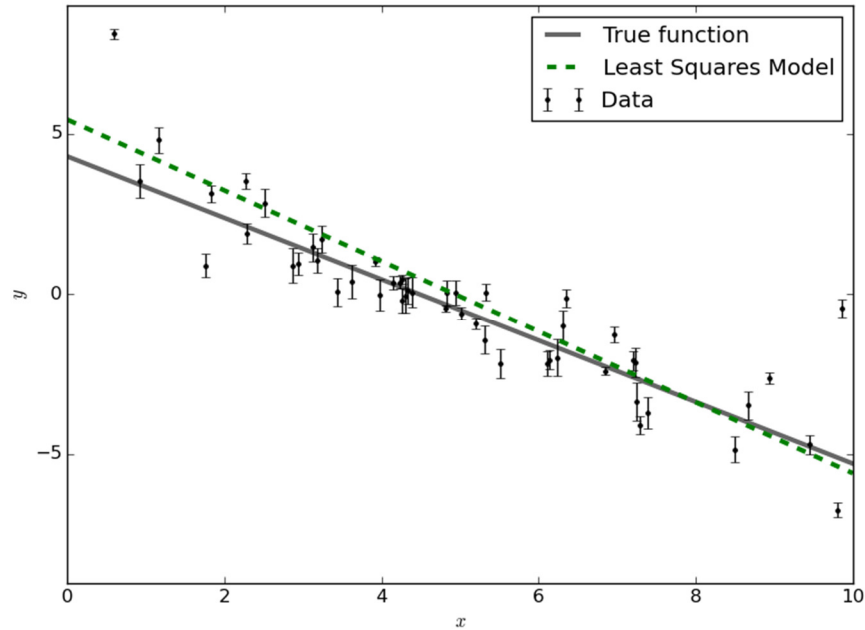


Figure 10: Sample data and the model generated by least squares regression. Parameter estimates are  $m_{ls} = -1.104 \pm 0.016$  and  $b_{ls} = 5.441 \pm 0.091$

Here, we see that the model has underestimated the slope and overestimated the intercept. A few unordinary data points have pushed the model away from the generating function, but this is by design of least squares regression; it penalizes large errors more and compensates to minimize them in the resultant model.

Another approach is to use maximum likelihood estimation. This involves employing the cost function in Equation. The quantity  $s_n^2$  underestimates the variance to account for the measurement uncertainty and provide an estimate for  $f$ .

$$\ln p(y | x, \sigma, m, b, f) = -\frac{1}{2} \sum \left[ \frac{(y_n - mx_n - b)^2}{s_n^2} + \ln(2\pi s_n^2) \right]$$

$$s_n^2 = \sigma_n^2 + f^2(mx_n + b)^2 \quad (7)$$

Finding the maximum of this function finds the parameter estimates that produce the maximum likelihood for generating the data. The log-likelihood is typically maximized for three reasons a) derivatives are simpler after logarithms are taken b) computer underflow is avoided and c) log is monotonically increasing, so finding the maximum log-likelihood solution is the same as the maximum likelihood solution. Figure 11 shows the results of this optimization.

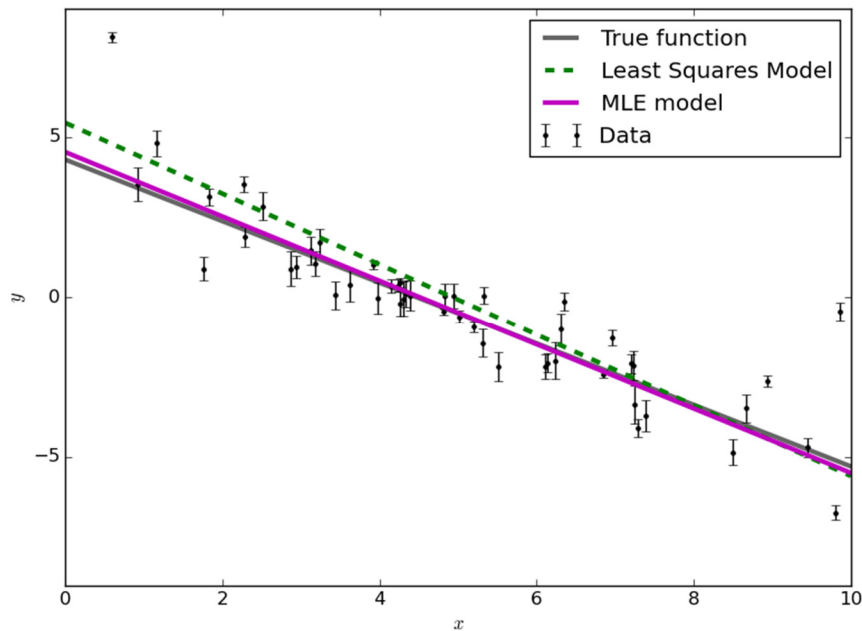


Figure 11: Sample data with the maximum likelihood model solution, in magenta. Parameter estimates are  $m_{mle} = -1.003$ ,  $b_{mle} = 4.528$  and  $f_{mle} = 0.454$ .

We will return to this data in the next section to see how Bayesian analysis produces a different result for parameter estimates.

## Chapter 3 – Bayesian Analysis

### Bayes' Theorem

Bayesian inference is an application of Bayes' theorem, Equation 8, which can be used to determine credible values for parameters in a model by considering them as probabilistic entities that have distributions.

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \quad (8)$$

Bayes' theorem specifies a relationship between the prior probabilities  $p(\theta)$ , the credibility of parameters without seeing the data  $D$ , the likelihood  $p(D|\theta)$ , the probability that the data was generated by the model with parameter values  $\theta$ , and the evidence  $p(D)$ , the overall probability of the data being created by the model, which is determined by averaging across all possible parameter values (because this is the same for any given parameter value, it is effectively a normalizing constant that can be ignored during optimization). Thus, by solving Bayes' theorem for a given set of observations and parameter values, we determine the posterior  $p(\theta|D)$ , the credibility of the parameters given the data [15].

In theory, we need to evaluate the equation for all possible values of  $\theta$  and generate full probability densities for the parameter space. For certain textbook-like applications, one can match up the likelihood function with a so called *conjugate prior* which produces a closed form parameterized distribution function as the posterior. For example, if we are modeling something with a binomial distribution  $Bi(n, p)$  and use a beta distribution  $B(\alpha, \beta)$  as our prior, the exact posterior is in the form  $B(s + \alpha, f + \beta)$  where  $s$  and  $f$  are the number of observed successes and failures, respectively.

For interesting real world applications, however, such as those of photolithographic models, no such solution exists and any integrable forms of the model are surely intractable. Additionally, the *curse of dimensionality* [16] makes it impossible to numerically map the complete parameter space in reasonable timeframe. Thus, we must explore the space of parameter values in the model in some informed fashion to locate those parameter values which represent the highest credible models.

### Markov chain Monte Carlo algorithms

To generate adequate estimations of the posterior distribution of the parameter space, a class of algorithms known as Markov chain Monte Carlo (MCMC) methods are used. Their properties are such that, if left to sample the parameter space to completion, they are guaranteed to generate the exact posterior distribution sought after, but can converge to a suitable approximation after some fraction of the number of iterations required to do so. In other words, the integrands of the algorithms are their equilibrium distributions.

MCMC algorithms work by a series of move proposals by so-called ‘walkers’ in the parameter space. Consider a two dimensional parameter space in  $a$  and  $b$ . The initial position for the walker is chosen randomly and the value of the likelihood function is evaluated at this position. Next, a new position is proposed by the algorithm (each one has a unique way of doing this proposal, which is what differentiates the algorithms). The likelihood function is evaluated at the proposed position in  $a$  and  $b$ , and this move is accepted or rejected based on the rules of the algorithm, but in general will be accepted when the likelihood of the new location is higher and rejected when it is not.

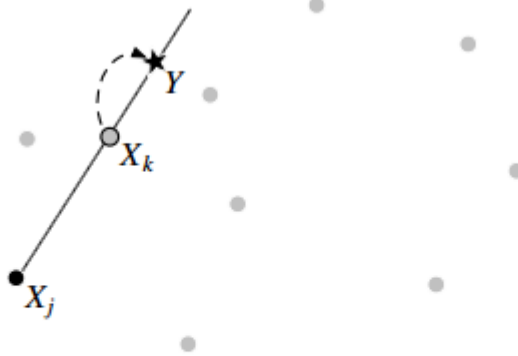
As each iteration continues, moves are proposed to a walker or walkers in the parameter space, and they converge to their equilibrium distribution; the posterior distribution that is an



estimation of the exact distribution created by the prior distributions, likelihood function and evidence created by Bayes rule, and we find the values of the parameters for our model that yield the post predictive model.

This work uses an algorithm known as the affine invariant ensemble sampler (AIES) which is based on work by Goodman and Weare [17]. As the name suggests, it uses an *ensemble* of walkers, not just one, that are each proposed moves simultaneously per iteration, which makes the algorithm efficient via the evaluation of many candidate models in parallel, important because the lithographic models in the study are relatively expensive to compute.

For a given ensemble of walkers, say 40, when move proposals are generated, the ensemble is divided into two sub-ensembles,  $j$  and  $k$ . For each walker in  $j$ , a walker in  $k$  is chosen to participate in a stretch move, which draws a line through the any-dimensional (due to the algorithm's affine-invariance) parameter space, plus an extension factor, to a new location,  $Y$ , as in Figure 12.



**Figure 2.** A stretch move. The light dots represent the walkers not participating in this move. The proposal is generated by stretching along the straight line connecting  $X_j$  to  $X_k$ .

*Figure 12: Figure with caption from Goodman and Weare's publication showing a stretch move [17]*

The amount of extension is drawn from a tunable distribution with scale parameter  $a$ , which can affect the convergence rate of the algorithm. Each walker in the ensemble gets a

move proposal in this manner, and, as in other MCMCs, the likelihood function is then evaluated at this location in the parameter space. The moves are accepted when the likelihood is higher and usually rejected if the likelihood is lower (some small random chance to accept a worse move is given to promote adequate exploration).

There are many diagnostics to evaluate whether or not the chains in the sampling are converged to an adequate sampling of the true posterior. This work invokes the Gelman-Rubin diagnostic as an estimate of  $\hat{R}$ , the potential scale reduction factor, which approaches 1.0 as sampling becomes complete [18].

### The Linear Model example, revisited

In the linear regression section, we explored finding parameter estimates for simple  $x$  by  $y$  data with uncertainties for each data point. Least squares regression and maximum likelihood were used to produce models that tried to estimate the true generating function for the data. Now that we have the power of Bayesian inference and MCMC algorithms, we can generate a posterior distribution of candidate models to describe the data.

First, we need a set of prior probabilities. For simplicity, we will use uniform distributions on  $m$ ,  $b$ , and  $\ln(f)$ . We also use the same likelihood function as the MLE model. Then, we will use the AIES with 100 walkers for 500 iterations to produce the posterior probabilities, shown in Figure 13. With these posterior probabilities generated, we can sample from them to generate a set of candidate models, shown in Figure 14. We can express the parameter estimates as the means of these distributions and use the 95% highest density interval (HDI) to quantify their uncertainty. Doing so, we come up with  $m_{ba} = -1.009_{-0.075}^{+0.077}$ ,  $b_{ba} = 4.556_{-0.353}^{+0.346}$  and  $f_{ba} = 0.463_{-0.063}^{+0.079}$ .

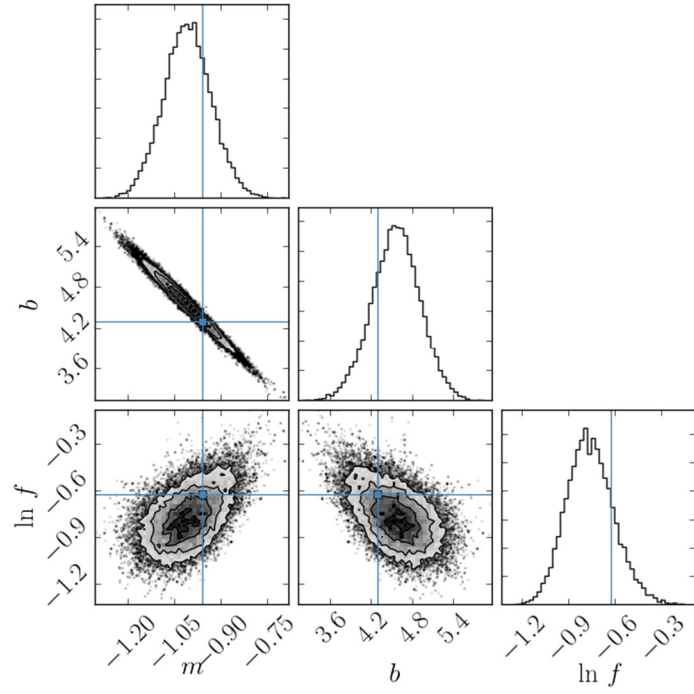


Figure 13: Posterior distribution for the parameters in the linear model. Top plots are 1D histograms, others are bivariate density plots. True values are shown in blue lines.

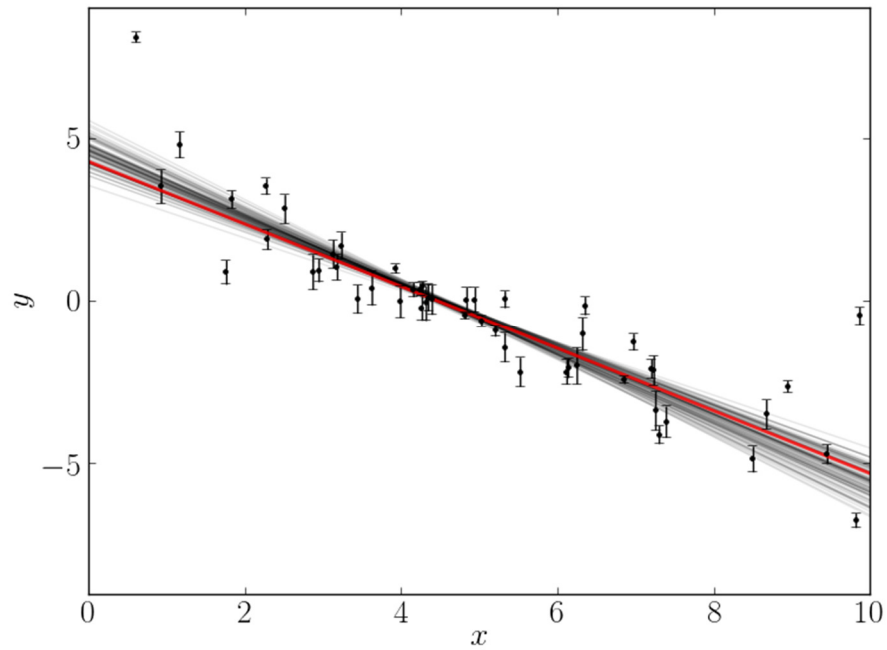


Figure 14: Red shows the true model. The rest of the lines are samples from the posterior distribution showing various candidate models. Bayesian analysis sees the solutions as a probabilistic entity.

## The Likelihood Function

Thus, to find the parameter values which achieve the highest credibility, we seek to use an MCMC algorithm to generate the posterior. However, first we consider some mathematical conveniences to make this task easier. First, we do not need to consider the denominator,  $p(D)$ , because it simply normalizes the entire function; if we maximize the posterior without this static quantity, we maximize it as if we had it, as well.

Secondly, taking the log of the function has several advantages: logarithm is a monotonic transformation which preserves the values of maximum likelihood and additionally simplifies the combination of probabilities to a sum of logarithms instead of a product of them, which is easier to differentiate. Finally, the actual values of each probability can be near zero, so underflow is avoided as we sum them instead of multiplying them together.

We then consider the sum of the prior probabilities, the likelihood of the value of the parameter at that iteration subject to its prior distribution, and the sum of the probabilities for each CD SEM measurement, each one subject to its unique shape parameters of a Student's  $t$ -distribution based on the count and standard deviation that yielded the measurement. Equation 9 describes the function we maximize under the MCMC algorithm.

$$\sum \ln pdf(\hat{\theta}|\theta) + \sum \ln pdf(e|v, \sigma) \quad (9)$$

Here,  $\hat{\theta}$  is the estimated value of  $\theta$  under the probability density function of that parameter's prior distribution. This work uses uniform and normal distributions as priors. The log-likelihood for the data is described as the sum of each CD measurements' error under a Student's  $t$ -distributed random variable. The probability density function for each is unique and depends on the measurement count and standard deviation information. The count, which describes the number of images taken to create the reported average CD value is used in the

degrees of freedom  $\nu$  and the shape parameter  $\sigma$  is taken from the standard deviation of that measurement. So,  $e$  is the error of that particular measurement (difference in measured and simulated CD values) and we calculate the probability of observing that error under the particular distribution that is unique to the measurement.

In this way, we give more credibility to measurements with less uncertainty than those with higher uncertainty, i.e., a gauge with many, tightly distributed measurements informs the likelihood more strongly than a gauge with few or spread out measurements. Maximizing this log-likelihood minimizes the difference between simulated and measured values, under the constraints of the model.

Figure 15 attempts to tie everything together. Recall that the ultimate goal of photolithographic models is for use in OPC – once a model is in place that will predict wafer CDs from a mask layout, OPC seeks to find mask solutions to produce the target contours on the wafer. An accurate model ensures that the solutions OPC finds will produce manufacturable contours on the wafer after the mask is produced.

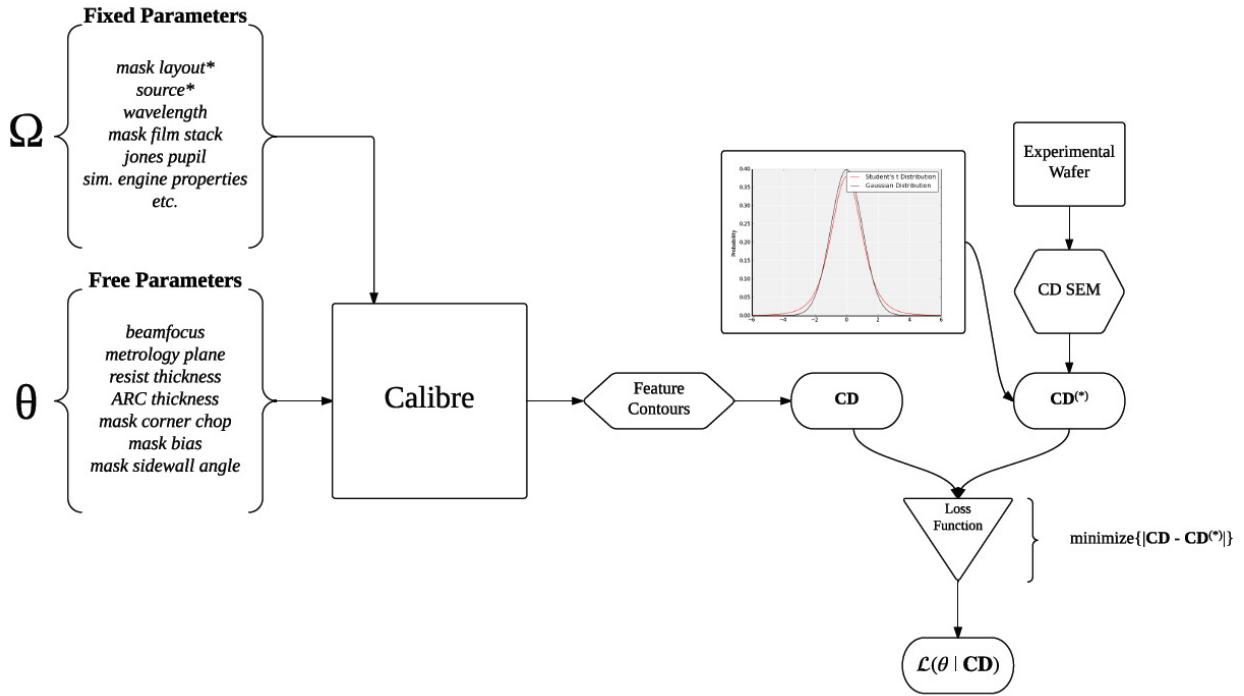


Figure 15: Flow diagram describing the goal of Bayesian analysis for photolithographic modeling. The model, which has fixed and free parameters, describe the photolithographic manufacturing process and produce simulated contours of the resist based on the mask layout. These are ideally as close as possible to the CD measurements from the wafer fab, which are shown to be drawn from a distribution due to stochastic effects.

## Implementation in Python

To implement a Bayesian inference scheme, Python™ [19] was used as a master control to connect the Calibre™ [20] simulation engine with the MCMC search algorithm. A script was written which takes in the components necessary for a simulation (simulation engine specifications, such as optical diameter and kernel count, wafer film properties, such as thickness,  $n$  &  $k$ ) and modifies a generic model specification file with the information. Before simulation, a 3D mask domain decomposition model (DDM) file is generated at the specified mask absorber sidewall angle by interpolating between two previously generated DDM at 80 and 90 degrees. Simulations performed here are using a constant threshold resist model which effectively models only the aerial image. No resist effects are considered for this work.

Each parameter in the model that is being optimized is accompanied by a prior probability which is defined by a chosen distribution (normal, uniform) and the shape parameters for that distribution. For example, resist thickness might be normally distributed around its nominal thickness with a standard deviation of 1nm. In many cases, these distributions must be truncated at certain values. It is unphysical and impossible to generate a DDM library at greater than 90 degrees, so these values must be forbidden (the cost function returns a negative infinity result for these cases). Table 1 shows each parameter in the model, its prior distribution and the truncated limits.

<i>Parameter</i>	<i>Prior Distribution</i>	<i>Truncated Limits</i>
Photoresist thickness	Normal( $\mu$ =nominal, $\sigma$ =1nm)	[0.8x, 1.2x nominal]
B/ARC thickness	Normal( $\mu$ =nominal, $\sigma$ =1nm)	[0.8x, 1.2x nominal]
Global mask bias	Normal( $\mu$ =0nm, $\sigma$ =0.5nm)	[-3, 3nm]
Mask cornerchop	Normal( $\mu$ =9nm, $\sigma$ =3nm)	[0, 20nm]
Absorber SWA	Normal( $\mu$ =85°, $\sigma$ =2°)	[80, 90]
Beamfocus	Uniform(-5nm, resist + 5nm)	N/A
Metrology plane	Uniform(0, resist thickness)	N/A

*Table 1: Parameters in the model along with their associated prior distributions and absolute limits. Beamfocus and metrology plane are relative to the top of the resist stack, such that 0 = top, and positive is into the plane of the wafer.*

The AIES used has a tunable number of *walkers* which are run in parallel. Thus, simulations at each point in the parameter space are run in parallel, which helps to conserve runtime. One of the disadvantages of the prototype is having to reinstantiate the Calibre™ simulation entirely each time, which does not allow for the benefit of caching certain parts of the simulation result (typically how the optimization routine is performed).

Once each simulation is complete, a file with the simulated CD values is generated, which is read by the master Python script and used to calculate the cost function for that set of parameters, which is equal to the sums of likelihoods in Equation 9. This cost function is then evaluated using the Python module `emcee` [21], which is an off-the-shelf implementation of the aforementioned AIES MCMC algorithm, to choose new sets of parameter values for each walker. This completes one iteration, and once the ensemble reports the values of the likelihood at the move proposals, which are either accepted or rejected, and a new set of move proposals are generated.

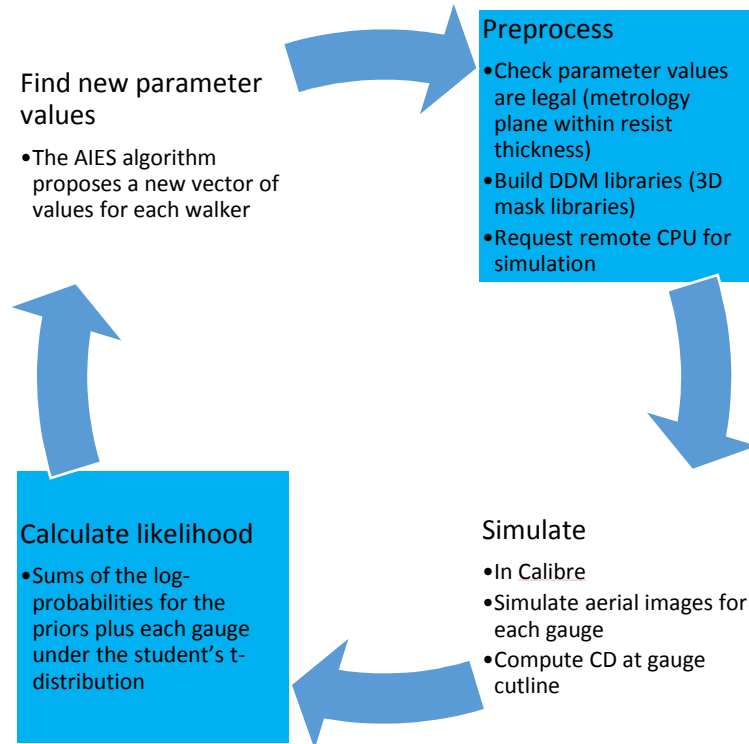


Figure 16: Flow diagram for generating the posterior distribution

The AIES was run with 40 walkers per calibration for 500 move proposals each, resulting in 20,000 iterations of simulations. While this number is far below what is typically done when running an MCMC algorithm, we are limited by the time it takes to perform each simulation, though it has been observed that convergence happens anyway during the



optimization. This may be due to the strong physical nature of the models in question such that the credibility of a random parameter vector is not high. This is observable in the posterior distribution plots as vast voids of exploration.

The testcases used were commercial datasets available to Mentor Graphics from their customers, and represented real calibration data used to create models for OPC on manufacturing reticles. Therefore, the data is anonymized wherever possible in this report, without specific parameter values or measurements where they could be traced to their source.

## Chapter 4 – Results and Analysis

### Initial, exploratory run

The end result of a MCMC algorithm is an estimation of the posterior distribution of the parameters in the model. For our case, this parameter space is in seven dimensions, which makes it difficult to completely visualize. However, we can observe each parameter's univariate posterior (averaging against all of the other parameters) and each possible bivariate distribution to see if there are any correlations between parameters. To do this, we construct a triangle plot shown in Figure 17, which contains a histogram for each parameter at the top of each column and a bivariate density plot for each pair of variables in the model. For parameters where it is appropriate, we also show the original, nominal value as a blue line.

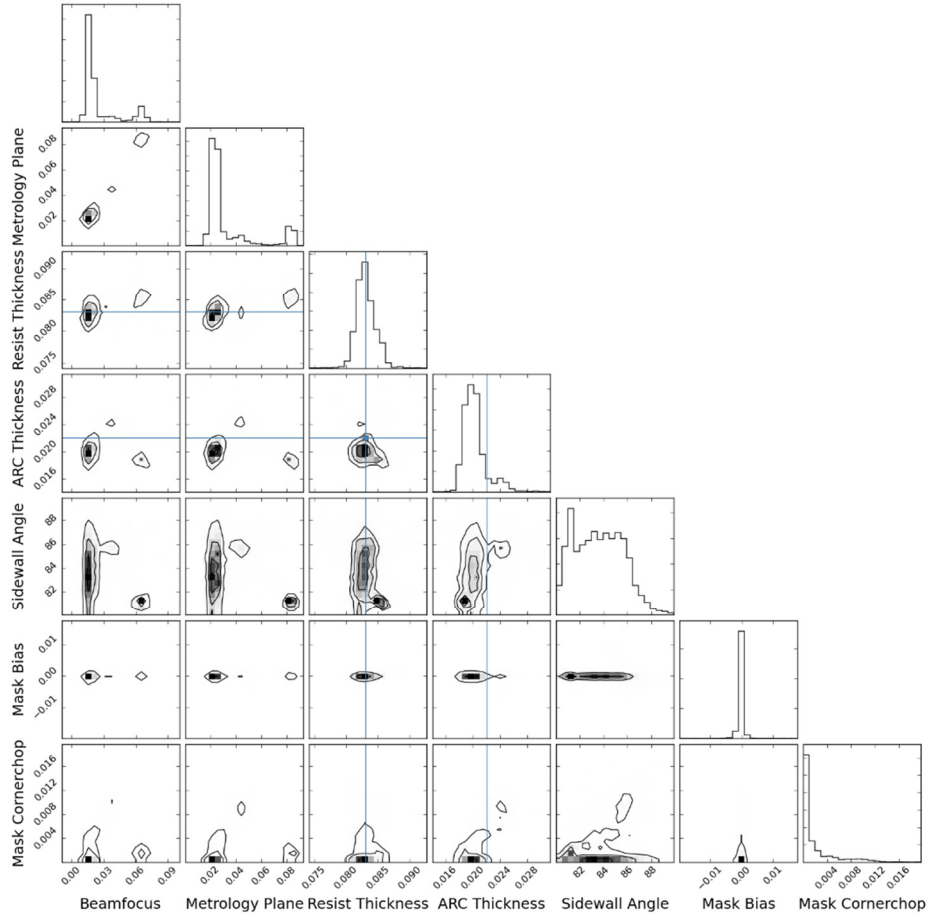


Figure 17: The seven dimensional posterior distribution using 100 gauges during the posterior maximization with AIES.

This early result shows an optimization using a small subset of the input gauges; typically datasets contain thousands of gauges, but in order to reduce the simulation time per iteration, only a random sampling of 100 was used to characterize the performance of the algorithm. For each parameter and bivariate plot, we can understand the responses in terms of modality and convergence or variance. For example, the mask cornerchop value is strongly converged to a unimodal response near 0 nm. Beamfocus, on the other hand, has two modes, one near the bottom of the resist and one near the top. This is a common signature in lithographic models and is an expected outcome from the effects of standing waves [22].

The sidewall angle has not converged and this could be caused by several different reasons: a) the MCMC algorithm has not finished adequately exploring solutions b) the parameter truly has large variance c) the parameter's value does not affect the cost function.

One thing to note is that the resist and ARC thicknesses have mostly converged to values with low variance, one of which matches the nominal input value and one that does not. Recall that, in general, the film parameters are simply given by the owner of the testcase and taken as truth. Here, we see that it is possible the uncertainties in these values lend other credible values than those given to us. The optimal ARC thickness in the model is 1 – 2nm different than the original value.

Does this mean that ARC thicknesses of the wafer or wafers used to produce the CDs in the test case was, indeed, 1 – 2nm thicker than reported? That is one possibility; others include that the variance across the wafer could be 1 – 2 nanometers or that the model simply performs better by adjusting this parameter to compensate for another effect. In this optimization we did not include the  $n$  &  $k$  of the resist or ARC, which could be different than their nominal values, but are being expressed as an equivalent change of thickness to change the optical path length for the photons through the wafer stack.

It is interesting to compare the posterior generated by this run to two other independent random samplings of 100 gauges from the master set, shown in Figure 18 and Figure 19.

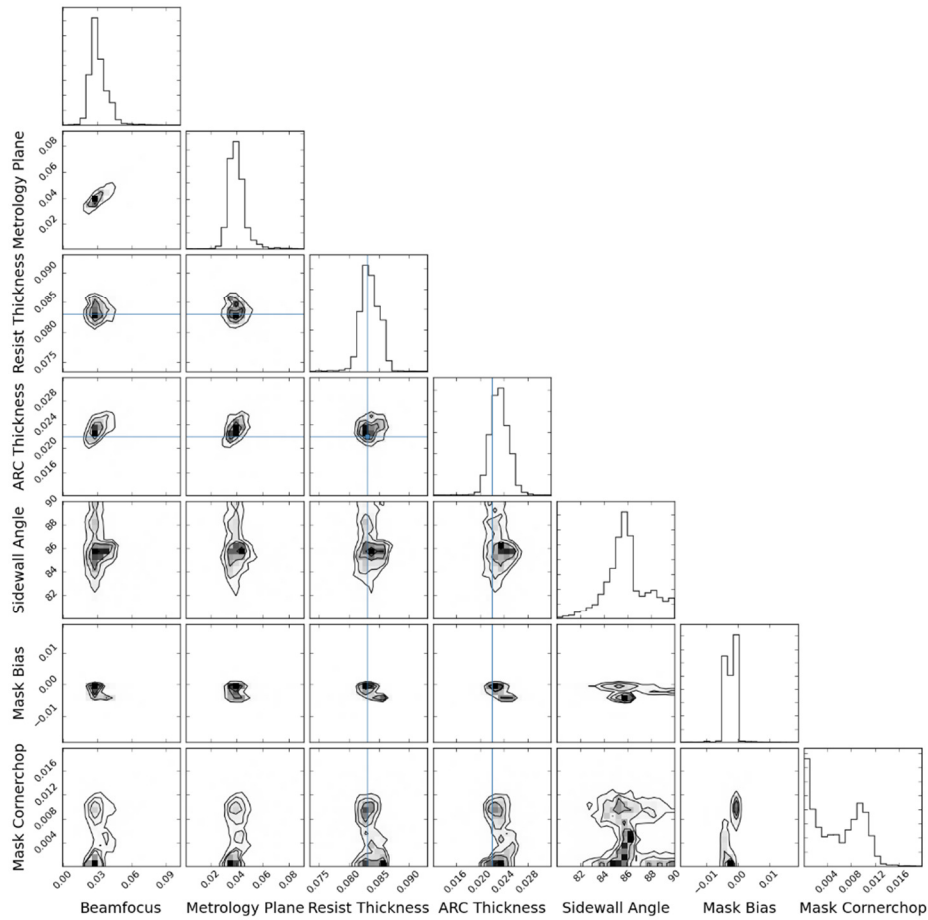


Figure 18: 2nd calibration from an independent random sample of 100 gauges from the master set.

Comparing the three subsets of data highlights potential biases in the data and vulnerabilities of certain parameters to feature type selection. Typically, gauge sets have thousands of gauges from a variety of feature types: pitch structures (1D line and space patterns), contact arrays, tip to tip structures, isolated lines, line end measurements, 2D logic structures, bulkhead structures and others. Generally, each feature type is parameterized in one or more dimensions of the feature, such as the line width or pitch of lines and spaces, and there will be a gauge to interrogate the CD at each combination.

When generating a random sample from the master set, it is possible that certain feature types end up excluded or over-represented compared to a different random sample. These biases will manifest in changes to the posteriors generated during an optimization for certain

parameters. Between these optimizations, we can see differences in values for mask bias, sidewall angle and mask cornerchop, which is explained by certain features' sensitivity to those parameters. For example, the sidewall angle of a mask absorber affects a line space pattern more than other feature types. Another example is that mask corner chop does not affect line space patterns (there are no corners near gauge sites in line space patterns).

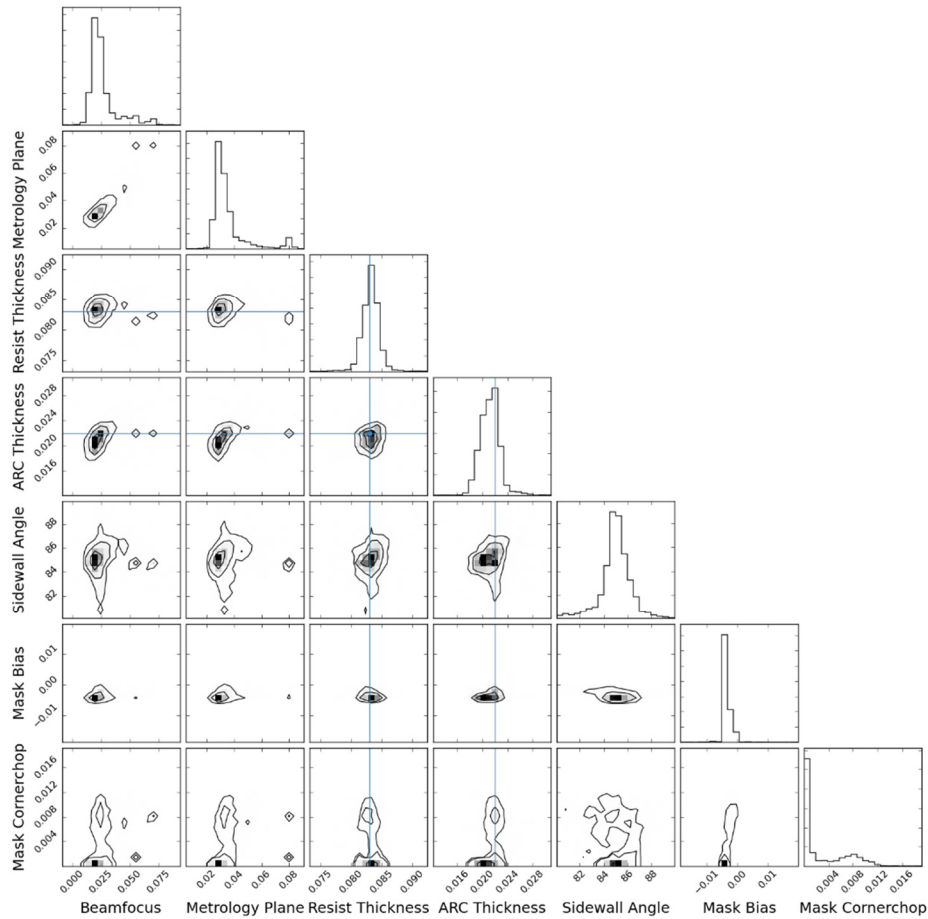


Figure 19: 3rd calibration from an independent random sample of 100 gauges from the master set

Resist thickness and beamfocus are invariant between the calibrations, which is expected and a sanity check that the algorithm is operating effectively. Other parameters have slight variations between the calibrations which could be due to subtle sampling biases in the data.

## Adding n & k of the resist and ARC

Given that early runs of the AIES to generate posteriors showed good convergence with 7 dimensions of parameters to explore, it was decided to add an additional 4 parameters, with accompanied prior distributions, to the model. In line with the thicknesses of the photoresist and ARC, the n & k of both films were added. These three parameters, thickness, n & k, represent the optical path length for photons traveling through the wafer stack during exposure (besides underlying films and the substrate) and help to capture a more complete representation of the physical processes during lithography. Table 2 shows the new parameters and their specifications in the model.

<i>Parameter</i>	<i>Prior Distribution</i>	<i>Truncated Limits</i>
Photoresist n	Normal( $\mu$ =nominal, $\sigma$ =2%)	[0.8x, 1.2x nominal]
Photoresist k	Normal( $\mu$ =nominal, $\sigma$ =2%)	[0.8x, 1.2x nominal]
B/ARC n	Normal( $\mu$ =nominal, $\sigma$ =2%)	[0.8x, 1.2x nominal]
B/ARC k	Normal( $\mu$ =nominal, $\sigma$ =2%)	[0.8x, 1.2x nominal]

*Table 2: The film stack properties added to the parameter space along with their priors and truncated limits*

Optical constants are the subject of much interest and uncertainty in the semiconductor industry and are typically produced from ellipsometry measurements that measure the transmission and reflectance and then fit a model to the data to extract n and k [23]. The accuracy of the resultant values from this procedure are dependent on very well calibrated measurement procedures. It is possible that these values are later verified in the fab with conditions that match those during manufacturing and data collection, but it is unknown to the author if this is typically carried out.

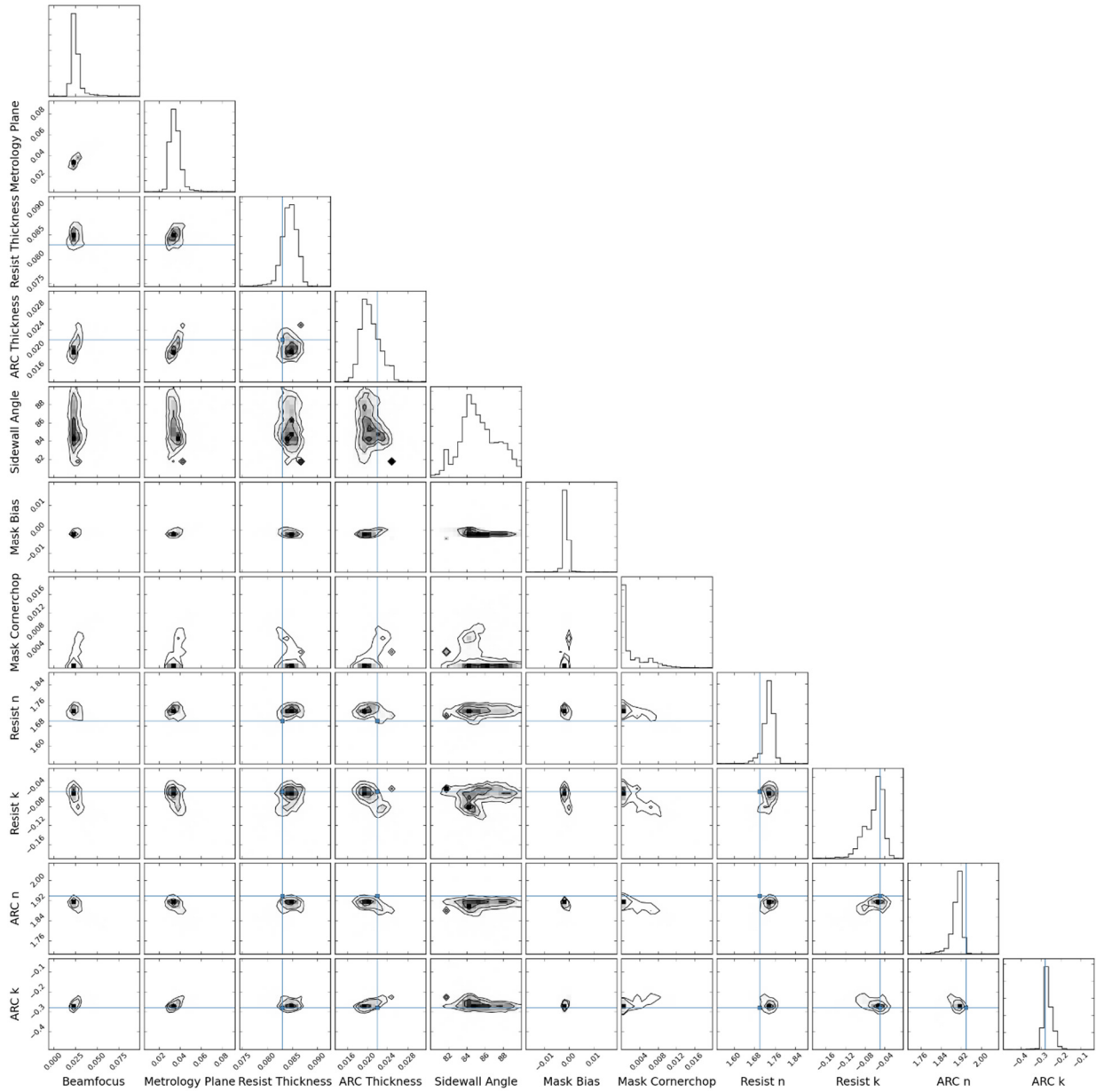


Figure 20: The full 11 dimensional posterior space. Blue lines indicate values given with the testcase for each parameter. Thus, differences between the given and posterior indicate the benefit from optimizing these parameters.

There are many interesting properties to observe in the posterior for this ‘full’ 11 dimensional optimization. Again, the main observations to make are: modality (uni- or multimodal), the standard deviation of individual parameters (seen mainly in the 1D histograms per parameter), any interactions between two parameters (seen in the 2D biplots) and where the posteriors’ convergence differs from the given values (blue lines).



All parameters in the posterior appear to have a unimodal response, indicating there is indeed one best value to describe the dataset (again, recall that the goal of Bayesian analysis is to find the parameter values which are most likely to produce the observed data under the given model and likelihood formation). Most parameters are strongly converged with small standard deviations, notable exceptions being the sidewall angle of the mask absorber and the ARC thickness.

Mask cornerchop has a minor interaction with most other parameters in the model for non-zero values, but the data seems to suggest zero is the most accurate. This is contradictory to the prior expectations for this parameter; recall that it was expected to have a nominal value of 9nm and a normal distribution about this value. This is an acceptable outcome under Bayesian analysis; priors will inform the posterior when the data does not, but if the data is conclusive then a prior may be overwhelmed.

Finally, we will consider the  $n$  and  $k$  of the wafer films; Figure 21 shows the posterior distributions for these in a magnified plot for convenience. Here, we can clearly see the optimization has found values not equal to the input values. Given that these parameters are typically excluded from optimizations, this is a significant result that shows better models exist when these parameters are not fixed. The values found by the analysis are different within the range of error for producing the values in the first place.

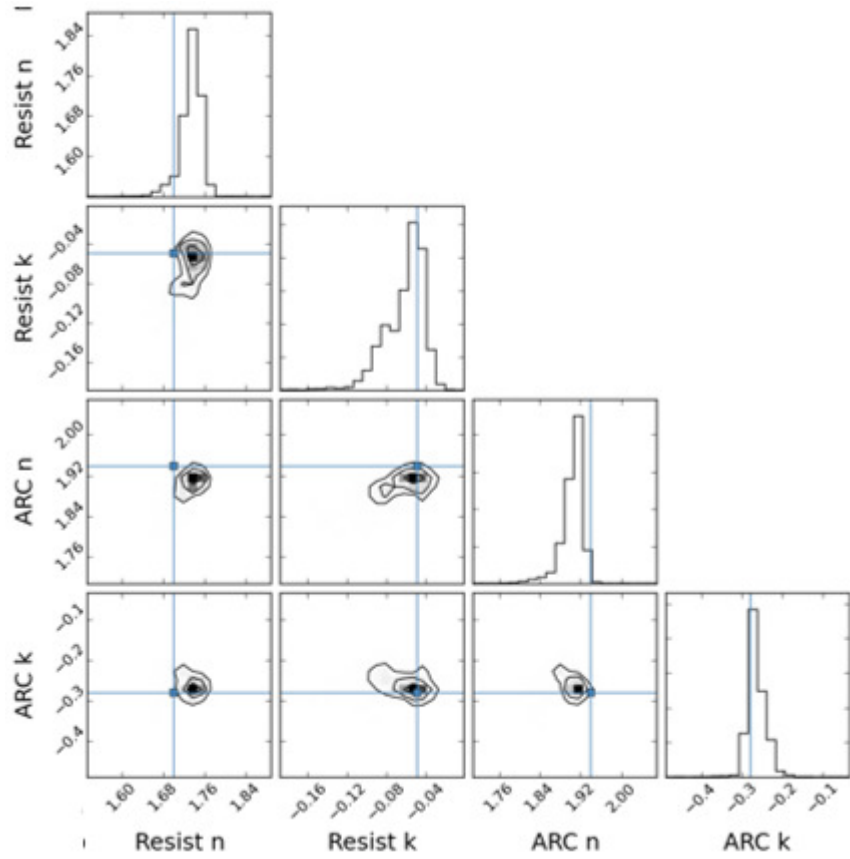


Figure 21: Magnified plot of the resist and ARC n & k posteriors

## Hierarchy in the Model

In the previous sections we used a simple one level model between our input parameters and the likelihood function. In this setup, each feature has a unique student's  $t$ -distribution that determines its contribution to the likelihood function directly. In a multi-level model, also known as model hierarchy, more complex schemes can be employed [15].

Consider, for example, modeling a coins from several different manufacturing sources with the goal of determining where each coin was made. Each manufacturer would have a distribution of Bernoulli  $\theta$  values their coins could be produced with. For example, Acme Coins Inc. might produce unfair coins with mean  $\theta$  of 0.2 while Fair Coins Inc. produces coins with mean  $\theta$  of 0.5. If we assume these  $\theta$  values are drawn from a normal distribution where  $\mu = \theta$  and unknown  $\sigma$ , we could estimate  $\sigma_{\text{acme}}$  and  $\sigma_{\text{fair}}$  for each coin in a sample of coins, as well as confidence intervals on where each coin was produced.

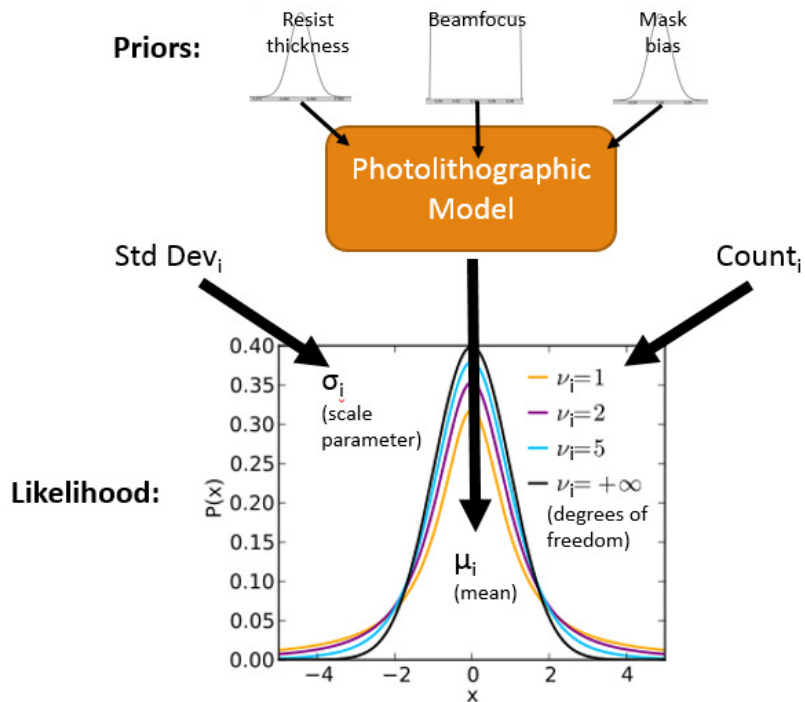


Figure 22: Graphical representation of the simple one level model hierarchy used so far.

We can do the same for our model. Figure 22 shows the original one level model hierarchy used in the previous sections. In order to make our model more informative, we might decide to group features into like categories. For example, typically 1D features, such as dense lines and spaces, behave differently than 2D features such as line ends. We might be able to understand how these features respond differently to parameters in our model by reworking the model hierarchy as shown in Figure 23.

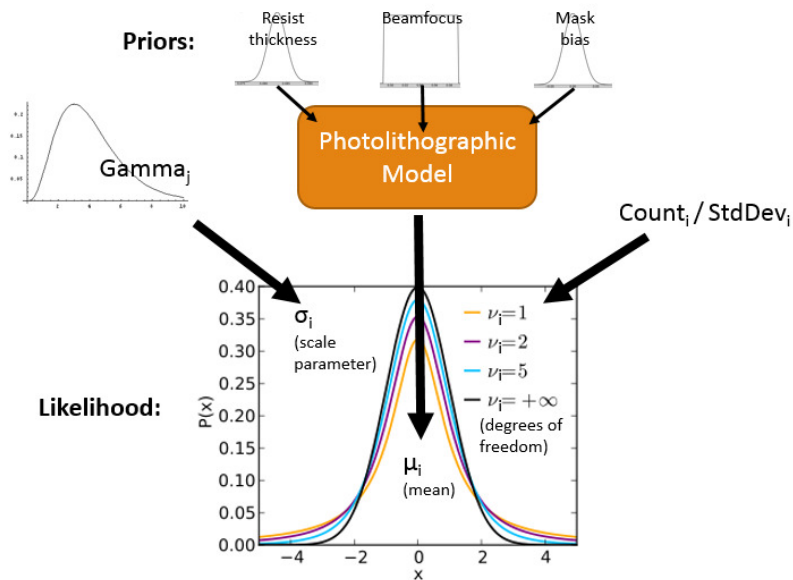


Figure 23: Graphical representation of two level model hierarchy using feature types to group the gauges.

For this, we will reassign the degrees of freedom,  $\nu$ , for each student's  $t$ -distribution to the number of measurements (count) divided by the standard deviation of those measurements (there is no requirement for  $\nu$  to be an integer) and the scale parameter  $\sigma$  will be drawn from a gamma distribution with fixed  $k$  and unique mean depending on which feature type the gauge is classified as.

Feature type groups were assigned by finding the five most common structure names (which are labels from the testcase owner) from all of the gauges and a 6<sup>th</sup> group for all other structures. The five grouped by structure named are assigned gamma distributions A-E and the

final with label O (to denote ‘other’). This was then run for an optimization lasting 250 iterations with 40 walkers to produce the posterior distribution shown in Figure 24, which has a total of 17 dimensions.

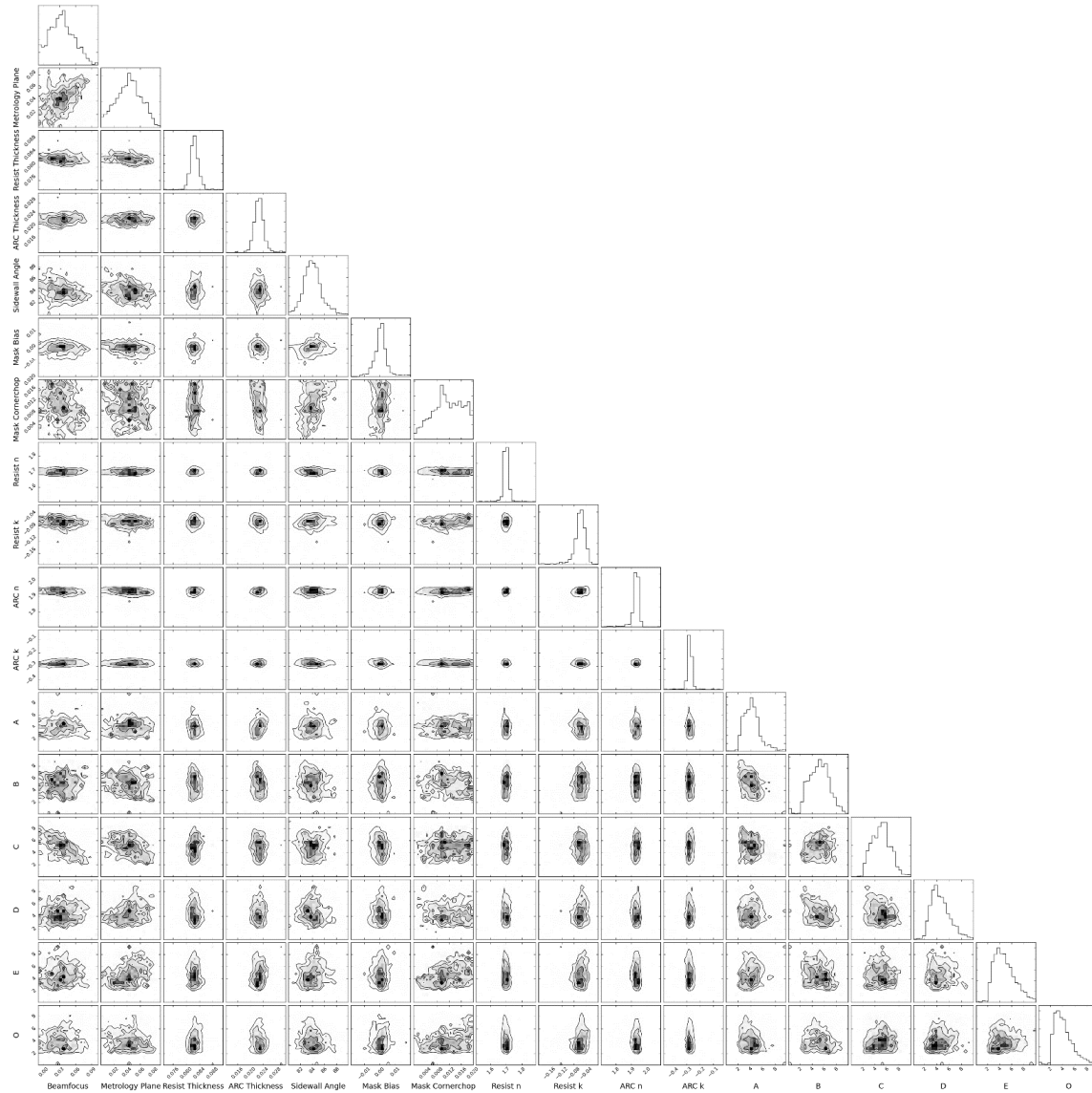


Figure 24: The posterior distribution triangle plot for the two-level hierarchical model and  $n$  &  $k$  film stack parameters.

The qualitative results for this optimization are not as well defined as the previous optimizations (large variances in most parameters) and the variances on the new gamma distribution parameters are especially high (lower right section in Figure 24). Generally, this has provided less information than the simple hierarchical model overall, which is not desired.

Because this optimization added six dimensions to the parameter space, it was hypothesized that this was finally too much for the AIES to estimate in the number of iterations that are available. To test this hypothesis, a second optimization was run using only the mask parameters and the grouping scheme parameters.

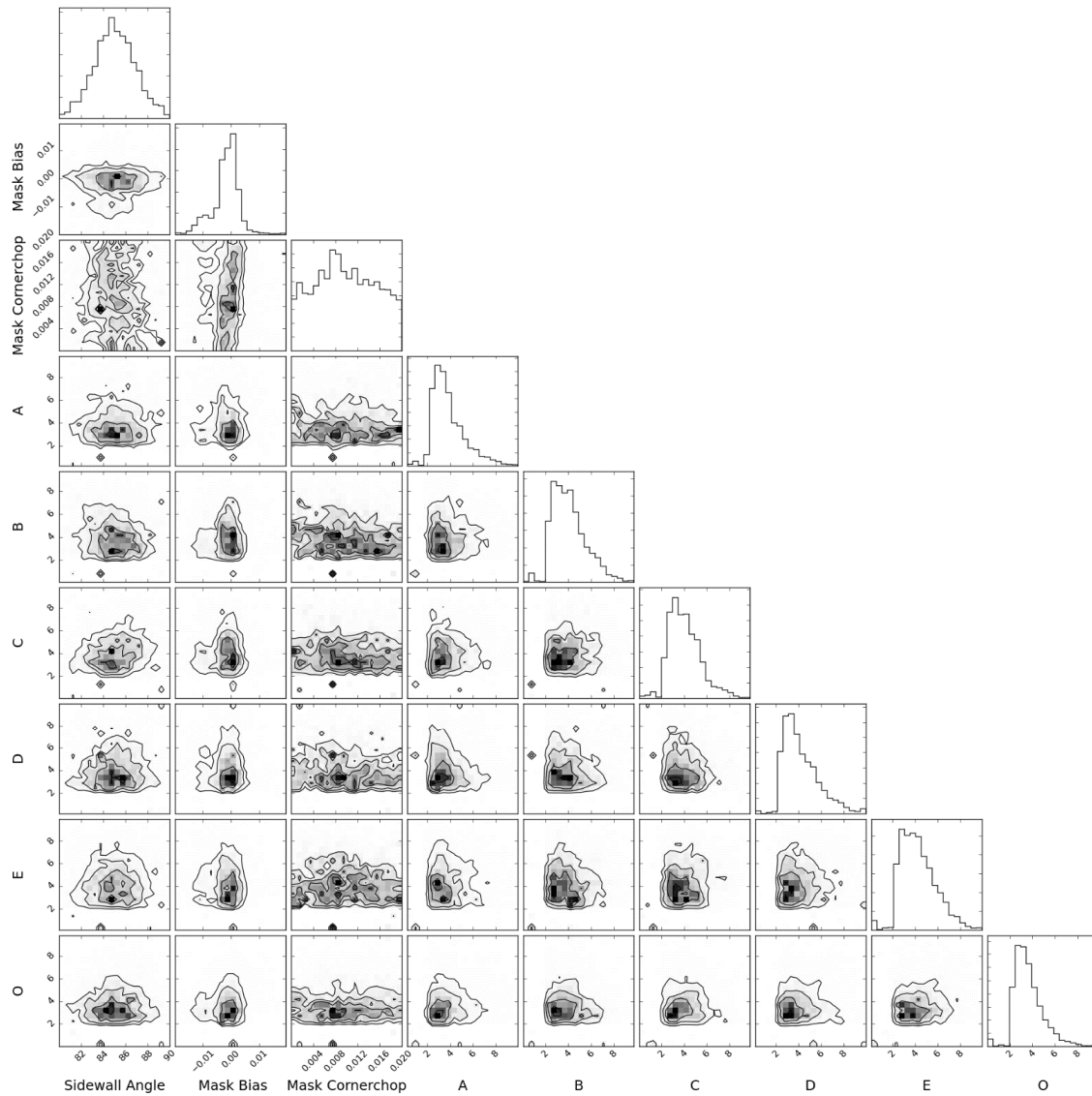


Figure 25: The posterior distribution triangle plot for the simple two-level hierarchical model.

However, this simplified scheme, too, shows the same high variance problem as the first test of hierarchy. There are several possible causes; a) the new likelihood formulation is simply not useful; the as defined gauge groupings are not meaningful to the data and simply obfuscate

meaningful parameter values, b) there does exist a good grouping scheme, but it requires a longer number of iterations to be informative or c) the hierarchical structure needs reformatting, perhaps with a different distribution to group both shape parameters in the student's  $t$ -distribution.

### The influence of prior distribution choice

A comparison was done to determine the difference between specifying different distributions as priors on the model parameters. Does the choice of prior distribution greatly influence the posterior distribution? In the general Bayesian case, the answer is certainly yes. Let us consider some scenarios to illustrate this point.

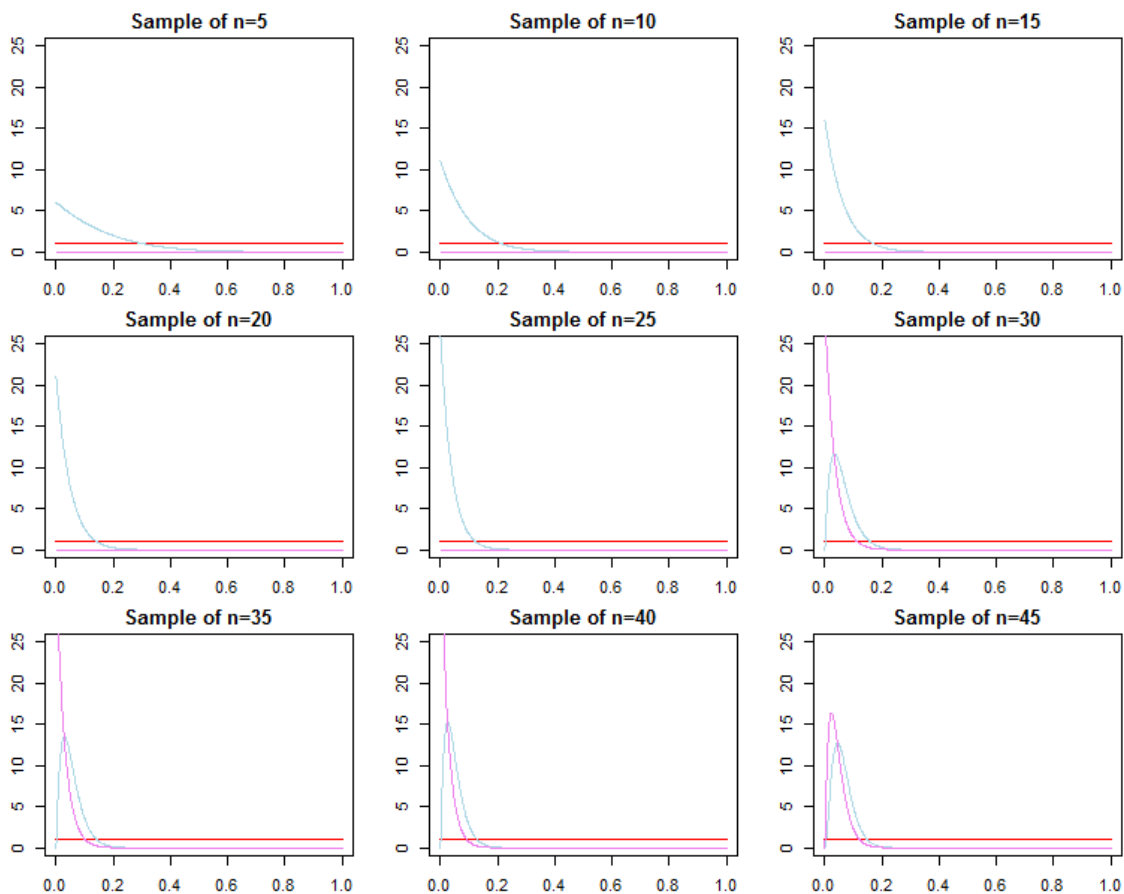


Figure 26: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a uniform prior. [24]

In Figure 26 the same model (prior and underlying data drawn for the likelihood) is in all 9 plots, which differ by the number of samples drawn to produce the likelihood estimate. We see that with a uniform (“uninformative”) prior, the posterior quickly matches the data. Contrast this result with the next two:

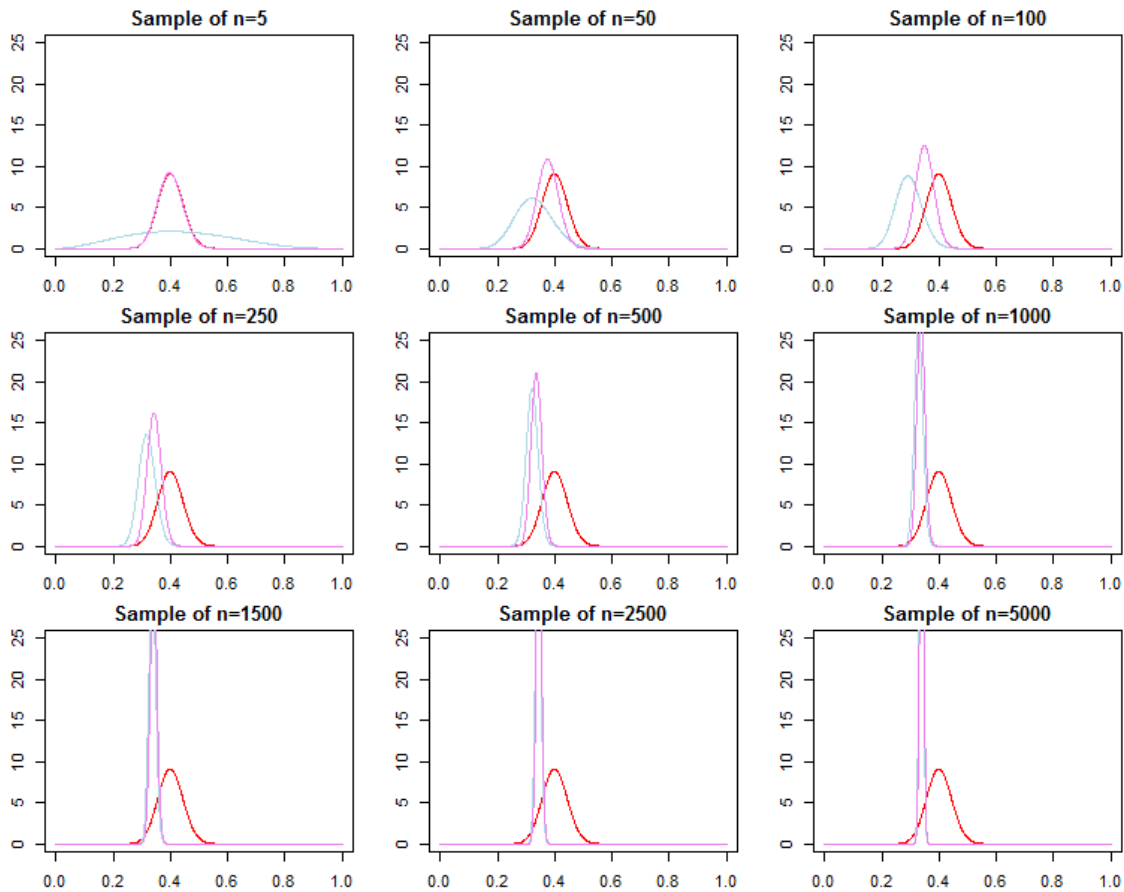


Figure 27: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a normal prior close to the likelihood. [24]

Here, the prior estimate is close to the likelihood; the data has a much smaller standard deviation and a different mean than the choice of prior and you need a much larger amount of data to overcome this than the uniform prior above, compare a sample size of 45 to over 500.



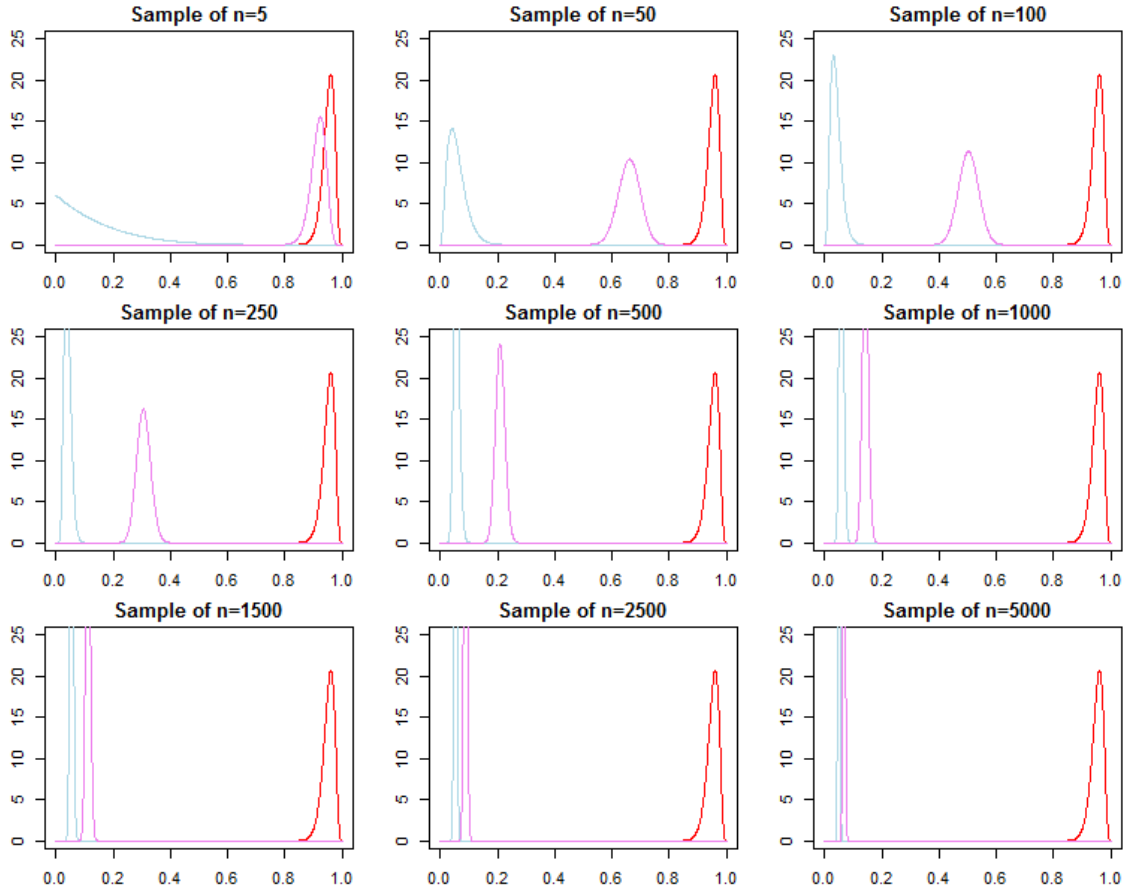


Figure 28: Priors (red), likelihoods (blue) and posteriors (violet) for various samples of identical true and unknown distribution with a prior far from the likelihood. [24]

Finally, in this example, the prior does not closely describe the likelihood at all. Here we see that the posterior doesn't resemble the likelihood until about 5000 samples.

So, we can see that the choice of prior can influence the posterior distribution, but it depends on how much *information* is contained between the prior and likelihood. So, in order to answer the question for our likelihood, we must do an experiment. For a small 100 gauge subset, mask bias, corner chop and sidewall angle were optimized once by using the normal distributions as priors from before and once by using uniform priors instead.

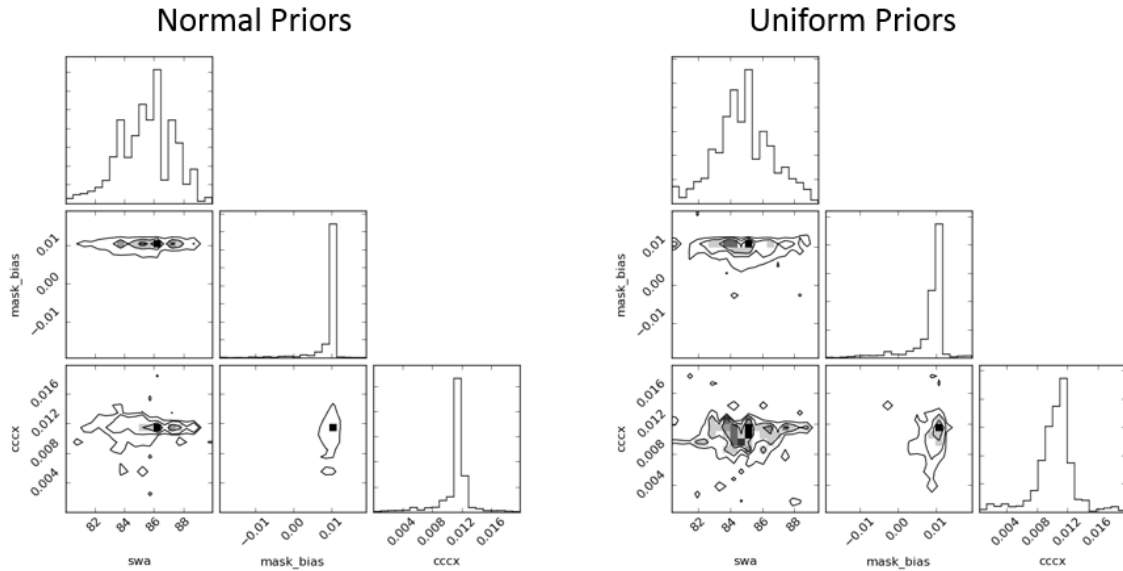


Figure 29: Posterior distributions for two optimizations on just mask parameters comparing the use of normally distributed priors to uniformly distributed priors.

Figure 29 shows this comparison, with a caveat: the normal prior case ran for about twice as many iterations due to an unforeseen issue, which has caused a difference in variance. In any case, we can see that the posterior distributions for each parameter are certainly converging toward the exact same values. This, therefore, means that the likelihood function contains a lot more information than the prior distribution.

When we consider the cost function formulation, this isn't too surprising. Recall Equation 9, which defines the posterior distribution as being generated by the sums of the logs of the prior distributions with the sums of the logs of *each* gauge's likelihood under the student's  $t$ -distribution. With sample sizes of at least 100 and typically in the several hundreds to thousands, it is clear that our likelihood contains a great deal more information than the priors. Thus, for this formulation, the exact prior distributions are not consequential.

## Posterior predictive checking and comparison to incumbent process

Finally, we consider the evaluation of the resulting posterior distributions and performing the so-called posterior predictive checks [25], [26], [27], [28]. In this scenario, we evaluate a sample of models from the posterior distribution on data not seen by the MCMC algorithm (a verification data set). Evaluating by sampling from the posterior distribution is typical for Bayesian inference and analysis in the statistical community, but has little use for an OPC model application; we cannot sample different parameter values as we simulate across the chip. However, it is still useful in a theoretical environment to evaluate the methodology.

	<b>Basic A</b>	<b>Basic B</b>	<b>Basic C</b>	<b>n &amp; k A</b>	<b>n &amp; k B</b>
<b>Mean</b>	5.391	4.913	5.39	5.008	5.339
<b>Variance</b>	0.171	0.085	0.133	0.101	0.253
<b>Median</b>	4.654	4.576	5.01	4.636	4.656
<b>Minimum</b>	4.061	4.146	4.039	3.832	3.966
<b>Maximum</b>	10.55	8.222	11.36	10.25	10.42

*Table 3: Comparison of nm RMS error between simulated models and wafer data for basic and complex models generated with different random samples of gauges. Compare to incumbent RMS minimization of 4.11*

Table 3 shows the comparison between five posterior predictive checks by evaluating 100 different models (selections of parameter values sampled from the posterior distributions). The basic models were without the n & k of the wafer film stack, while the other two models contained these variables. We compare these results to those obtained by the incumbent process, which is simple RMS minimization using a gradient-descent-like search algorithm.

We can draw several conclusions from these results. Perhaps most importantly, the Bayesian inference methods are capable of providing models which are more accurate than the incumbent process, notable by the minimum RMS values observed – we would undoubtedly choose these models for full chip wafer OPC over the incumbent model. Secondly, the

optimization of  $n$  &  $k$  does, as noted in earlier sections, provide a benefit over not doing so, even in this evaluation schema.

Finally, we observe fairly large variances and ranges for all of the evaluations. This would likely be reduced if the posterior was allowed to generate for more iterations, thereby reducing the variances of the parameters themselves, but overall the results are reasonable and consistent.

## Conclusions

This work has successfully demonstrated the use of Bayesian analysis and inference methods to produce more accurate models of photolithographic processes by including uncertainty in model parameters and model training data. We have shown that the use of a MCMC search algorithm coupled with a well-defined cost function, constructed of a prior and a likelihood informed by probabilistic representations of wafer data. We have also shown that, instead of using the given values for film stack optical parameters  $n$  &  $k$ , it is possible to find more descriptive models by tuning these parameters.

The results established in this work are relevant in several ways to the industry of photolithography and the modeling thereof. Firstly, they expand upon the use of Bayesian analysis to a domain that has not yet widely adopted it. Secondly, they improve upon the process of record by demonstrating improved accuracy at minimal cost.

Multilevel hierarchy was explored, though without much success, by adding gauge groupings to control a shape parameter of the student's  $t$ -distribution of each gauge as drawn from a gamma distribution. We also showed that the particular distribution of the priors is not relevant for this, thus indicating that a richly informational likelihood was formulated.

Finally, we showed through posterior predictive checking that the models generated from the posterior distributions are useful models that are capable of better predictions than those produced by the incumbent process. By using more of the information available to modelers, we show an improved and more accurate model that could be used to perform OPC that ultimately has fewer hotspots (wafer errors missed by the model) and require fewer reworks.

## References

- [1] I. Roadmap, 2015. [Online]. Available: <http://www.itrs2.net/itrs-reports.html>.
- [2] Z. Deng, C. Du, L. Hong, L. Zhang and J. Wang, "An efficient lithographic hotspot severity analysis methodology using Calibre PATTERN MATCHING and DRC application," in *Proc. SPIE 9427, Design-Process-Technology Co-optimization for Manufacturability IX*, San Jose, California.
- [3] L. Rayleigh, "On the Theory of Optical Images, with special reference to the microscope," *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, vol. 42, no. 5, pp. 167-195, 1896.
- [4] J. Sturtevant, E. Tejnil, T. Lin, S. Schultze, P. Buck, F. Kalk, K. Nakagawa, G. Ning, P. Ackmann, F. Gans and C. Buergele, "The impact of 14-nm photomask uncertainties on computational lithography solutions," in *Proc. SPIE 8683, Optical Microlithography XXVI*, San Jose, California, 2013.
- [5] B. W. Smith, A. Bourov, H. Kang, Y. Cropanse, Y. Fan, N. Lafferty and L. Zavylova, "Water immersion optical lithography at 193 nm," *Journal of Microlithography, Microfabrication and Microsystems*, vol. 1, no. 3, pp. 44-51, 2004.
- [6] K. Ronse, P. De Bisschop, A. M. Goethals, J. Hermans, R. Jonckheere, S. Light, U. Okoroanyanwu, R. Watso and D. McAfferty, "Status and critical challenges for 157-nm lithography," *Microelectronics Engineering*, vol. 1, no. 3, pp. 44-51, 2004.
- [7] K. Lai, *Computational basis for Advanced Lithography Techniques*, Course materials, 2016.
- [8] R. Guerrieri, K. H. Tadros, J. Gamelin and A. R. Neureuther, "Massively parallel algorithms for scattering in optical lithography," *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 10, no. 9, pp. 1091-1100, 1991.
- [9] A. Neureuther and A. K. Wong, "Rigorous Three-Dimensional Time-Domain Finite-Difference Electromagnetic Simulation for Photolithographic Applications," *IEEE Trans. Semiconductor Manufacturing*, vol. 4, no. 8, pp. 419-431, 1995.
- [10] K. D. Lucas, H. Tanabe, C. M. Yuan and A. J. Strojwas, "Efficient and Rigorous 3D Model for Optical Lithography Simulation," *Proc. SIS, Simulation of Semiconductor Devices and Processes*, pp. 14-17, 1995.
- [11] N. Cobb, *Sum of Coherent Systems Decomposition by SVD*, University of California at Berkeley, Department of Electrical Engineering and Computer Science, 1995.
- [12] K. Adam, *Domain Decomposition Methods for the Electromagnetic Simulation of Scattering from 3D Structures with Applications in Lithography*, Berkeley: University of California, Berkeley, 2001.
- [13] M. L. Konstantinos Adam, "Hybrid Hopkins-Abbe method for modeling oblique angle mask effects in OPC," in *Proc. SPIE 6924, Optical Microlithography XXI*, San Jose, California, 2008.
- [14] Y. Granik, D. Medvedev and N. Cobb, "Toward standard process models for OPC," in *Proc. SPIE 6520, Optical Microlithography XX*, San Jose, California, 2007.

- [15] J. K. Kruschke, *Doing Bayesian data analysis : a tutorial with R, JAGS, and Stan*, Burlington, MA: Academic Press, 2014.
- [16] T. Hastie, R. Tibshirani and J. Friedman, "Local Methods in High Dimensions," in *The Elements of Statistical Learning*, Springer, 2009, pp. 22-27.
- [17] J. Goodman and J. Weare, "Ensemble samplers with affine invariance," *Communications in Applied Mathematics and Computational Science*, vol. 5, pp. 65-80, 2010.
- [18] A. Gelman and D. Rubin, "Inference from iterative simulation using multiple sequences," *Statistical Science*, vol. 7, pp. 457-511, 1992.
- [19] *Python*, <http://www.python.org>.
- [20] *Calibre WORKBench*, Mentor Graphics.
- [21] D. Foreman-Mackey, D. W. Hogg, D. Lang and J. Goodman, "emcee: The MCMC Hammer," *Publications of the Astronomical Society of the Pacific*, vol. 125, pp. 306-312, 2013.
- [22] Y. Fan, C.-E. R. Wu, Q. Ren, H. Song and T. Schmoeller, "Improving 3D resist profile compact modeling by exploiting 3D resist physical mechanisms," in *Proc. SPIE 9052, Optical Microlithography XXVII*, San Jose, California, 2014.
- [23] F. Padera, "Measuring Absorptance (k) and Refractive Index (n) of Thin Films with the PerkinElmer Lambda 950/1050 High Performance UV-Vis/NIR Spectrometer," 2013. [Online]. Available: [http://www.perkinelmer.com/lab-solutions/resources/docs/APP\\_Thin-films.pdf](http://www.perkinelmer.com/lab-solutions/resources/docs/APP_Thin-films.pdf). [Accessed 2017].
- [24] Tim, "Cross Validated -- Do Bayesian priors become irrelevant with large sample size?," 2016. [Online]. Available: <https://stats.stackexchange.com/questions/200982/do-bayesian-priors-become-irrelevant-with-large-sample-size>.
- [25] D. J. Spiegelhalter, "Incorporating Bayesian ideas into health-care evaluation," *Statistical Science*, pp. 156-174, 2004.
- [26] A. Gelman, J. B. Carlin, H. S. Stern and D. B. Rubin, *Bayesian data analysis*, Chapman & Hall, 2004.
- [27] A. Gelman and J. Hill, *Data analysis using regression and multilevel/hierarchical models*, Cambridge University Press, 2006.
- [28] A. Gelman, X. L. Meng and H. Stern, "Posterior predictive assessment of model fitness via realized discrepancies," *Statistica sinica*, pp. 733-760, 1996.