Bayesian Optimization for Signal Transmission Including Crosstalk in a Via Array

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***Abstract*—Signal integrity is becoming an important aspect of EMC engineering of digital systems. The signal integrity performance of printed circuit board links is influenced by a large number of design choices. Bayesian Optimization is a method that can optimize a large number of parameters in a reasonable amount of time. In this work it is shown that Bayesian Optimization can be used for the optimization of interconnect models with respect to their transmission and crosstalk performance. The first example is the optimization of the transmission of a single via. The second example is a 10 by 10 via array where the optimization includes transmission and crosstalk. The results obtained with the Bayesian Optimization are compared with the results of a Genetic Algorithm and with design guidelines derived from a physical perspective.**

I. Introduction

Modern high-speed links require a careful selection of design parameters to achieve a high performance. These design parameters, which could be part of the printed circuit board (PCB) or the I/O, are not independent of each other. To achieve a good performance, usually several iterations of parameter tuning are required. Furthermore, one parameter change can have multiple effects that could contradict each other.

Several works have studied the use of optimization for the design process. One common method is the Genetic Algorithm (GA). It can be used for a multitude of problems in SI/PI [1], [2]. While this method is widely used, it requires a lot of evaluations of the optimization function. This can render GA too time-consuming. Another optimization technique that has become popular is the Bayesian Optimization (BO) [3], [4]. This method aims to minimize the number of function evaluations, which enables its use with time-intensive simulations. Due to their complex parameter dependencies, high-speed links could benefit from an efficient optimization method. This work investigates the applicability of BO to the design of digital links on printed circuit boards (PCB's). The results of the optimization are compared with design guidelines that are derived through the link physics. The first link example is a single via in a multilayer PCB and the second link is a via array that includes multiple traces. Fig. 1 shows an example of link elements that are also present in the via array link model. The design objectives are the transmission between the via and the stripline port as well as the far-end crosstalk (FEXT). A similar link has already been studied in [5], [6]. The optimization goals that are considered are the differential transmission and the differential crosstalk. Both are represented by a weighted power sum to simplify the analysis. The optimization results are compared with a Genetic Algorithm. The results can also be interpreted from a physical perspective based on the knowledge about the parameter dependencies of a printed circuit board link.

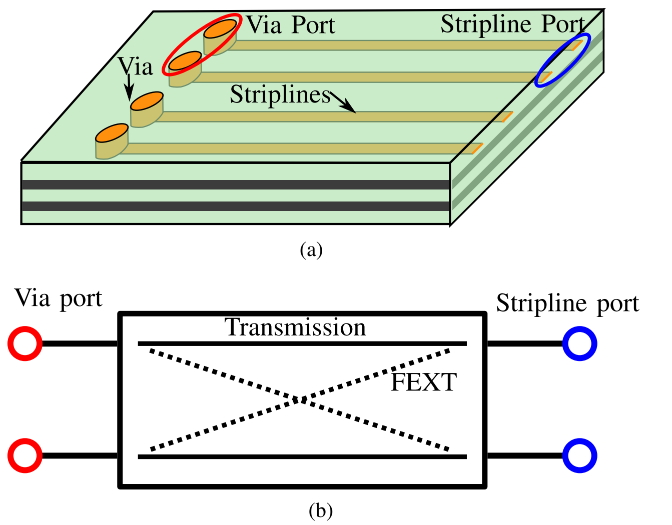

Fig. 1. Typical elements of a printed circuit board link. Similar elements can also be found in a via array link. The transmission and the crosstalk are the object of the optimization. (a) Schematic link model. (b) Block diagram of parameters of interest.

II. Modeling Approach and Figures of Merit

The link models are simulated with the physics-based via modeling [7] in a frequency range between 1 and 100 GHz. This method is considerably faster than 3D full-wave methods. Instead of a 3D simulation, the parallel-plate impedance of the PCB is simulated based on a 2D approach, the contour integral method [8], and then combined with the near-field model of the via. The striplines are simulated based on a 2D boundary element approach. A multilayer PCB can be simulated by concatenating the results of each dielectric cavity. The correlation of this method with full-wave methods up to 100 GHz can be found in [6]. Fig. 2 shows the S-parameters

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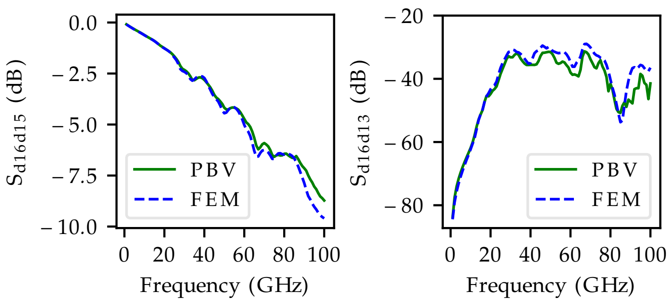


(a) (b)

Fig. 2. S-parameters of the array model shown in Fig. 3, obtained with the finite element method (FEM) and the physics-based via modeling (PBV). (a) Differential transmission between ports 16 and 15. (b) Differential far-end crosstalk between port 16 and 13.

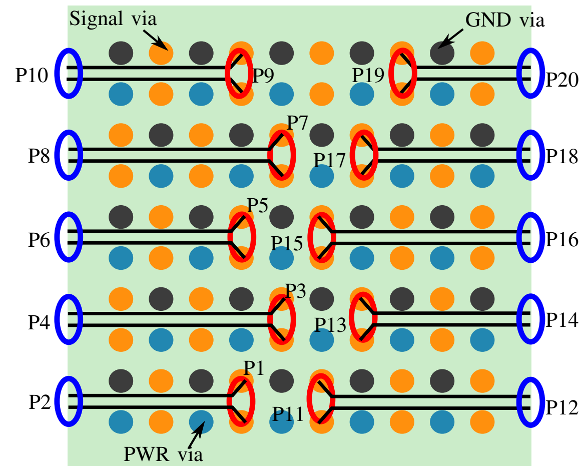


Fig. 3. Top view on the via array link. The differential ports are indicated on the vias (red) and at the end of the striplines (blue). Signal vias are shown in orange, GND vias in gray, and power vias in blue. The stack-up is shown in Fig. 4(c).

for the via array model shown in Fig. 3, simulated with FEM and the physics-based via modeling. Very good correlation can be observed for the transmission and the crosstalk.

The optimization process requires a clearly defined objective function. There are different ways to derive a figure of merit (FOM) from S-parameters that fulfill this condition. One possible FOM is the eye opening of an eye diagram. The advantage of eye diagrams is their capability to represent a large number of effects, both from the passive channel itself as well as from the I/0 design, e.g. equalization and line coding. The disadvantage is that they require an additional time domain simulation which increases the total simulation time.

Figures of merit that are defined in frequency domain are convenient because the additional time domain simulation is not required. This work focuses on the passive channel and a FOM should be able to represent both transmission and crosstalk effects. One possibility is the integrated crosstalk noise [9]. Another frequency domain FOM, the weighted power sum, was proposed in [10], [11]. The weighted power sum of crosstalk at port i is defined as:

$$WPSXT_i = \sqrt{\sum_{k=1}^{N_f} \left(\sum_{j=1;j\neq i}^{N_p} |FEXT_{i,j}(f_k)|^2 \right) \cdot |w(f_k)|^2} \tag{1}$$

N_f is the number of frequency points, N_p is the number of crosstalk aggressors. $FEXT_{i,j}$ is the FEXT S-parameter entry between ports i and j. w is the spectrum of the applied digital signal which can be calculated from the Fourier transformation of a pseudo-random bit sequence. f_k is the frequency vector. A similar weighted power sum of transmission (WPT) can be calculated by setting N_p to 1 and using the transmission S-parameter entry instead of the FEXT. These can be divided to calculate a signal to crosstalk ratio (WSXTR) [12].

III. Bayesian Optimization Approach

Bayesian Optimization (BO) [13] is a black-box optimization technique that requires few evaluations of the objective function. Recent research has focused on the extension to high-dimensional problems [14]. The goal is to find x^* to maximize the unknown objective function $f(x)$.

$$x^* = \arg\max f(x) \tag{2}$$

Two elements are necessary for the optimization process: A probabilistic surrogate model of f and an acquisition function to select the n query points $x_{1:n}$. One possibility to define a surrogate model is a Gaussian Process (GP) with a mean μ and a covariance matrix K.

$$f(x) \sim \mathcal{N}(\mu(1:n), K_{1:n}) \tag{3}$$

In this example the mean is constant which makes the model non-parametric. The covariance matrix can be constructed from a known kernel function such as a Matérn 5/2 kernel. To find the evaluation points that would maximize the knowledge about f an acquisition function u is defined and evaluated. The next evaluation point of f is chosen such that the acquisition function is maximized. Typical functions are probability of improvement (PI), expected improvement (EI), and upper confidence bound (UCB) [13], [15]:

$$u_{PI} = \Phi\left(\left(\mu(x) - \tilde{f}^* - \zeta_{PI}\right)/\sigma(x)\right) \tag{4}$$

$$u_{EI} = \left(\mu(x) - \tilde{f}^* - \zeta_{EI}\right)\Phi(Z) + \sigma(x)\phi(Z) \tag{5}$$

$$u_{UCB} = \mu(x) + K\sigma(x),\ K = \sqrt{2\ln(2\pi M^2/(12\eta_{UCB}))} \tag{6}$$

where Φ and ϕ are the CDF and PDF of the normal distribution and $Z = \left(\mu(x) - \tilde{f}^* - \zeta_{EI}\right)/\sigma$. M is the number of calls made to the UCB. The acquisition function is alternated with every iteration of the optimization and all three are used in this work. ζ_{PI}, ζ_{EI}, and η_{UCB} are tunable hyperparameters of the optimization.

If f is multidimensional such that $x \in X^d$, more function evaluations are required to predict f with sufficient accuracy.

Table I
HYPERPARAMETER COMBINATIONS FOR THE BAYESIAN OPTIMIZATION. THE GROUP DISTRIBUTIONS DEPEND ON THE LINK MODEL.

	A	B	C	D
Groups Single Via Model	4,3	5,2	5,2	4,3
Groups Array Model	7,5	8,4	8,4	7,5
$\eta_{\mathbf{UCB}}$	0.03	0.03	0.05	0.05
$\zeta_{\mathbf{EI}}$	0.2	0.2	0.1	0.1
$\zeta_{\mathbf{PI}}$	0.2	0.2	0.1	0.1

This decreases the speed of the optimization. A simplification is possible if the function f can be decomposed into additive subparts:

$$f(x)=\sum_{i=1}^{d} f_i(x_i)+\sum_{1<i<j<d} f_{ij}(x_i,x_j)+\sum_{1<i_1<i_n<d} f(x_i,...,x_n) \quad (7)$$

n is the number of allowed interactions. This allows the use of an additive kernel which can be constructed from the subkernels of the individual parameters $x^{(i)}$. The basis for that is the Matérn 5/2 kernel. One promising method to select the query points of f is a Deep Hierarchical Partitioning Tree (DPT) [15]. A sensitivity is calculated for each parameter of f and the parameters are combined into groups of descending sensitivity. The tree is at first expanded vertically by splitting the sample space along each group to create multiple hypercubes $H_{t,k}$. Candidate point $c_{t,k}$ from this hypercube is the arithmetic mean of minimum and maximum of this hypercube. To increase the exploitation of promising regions a horizontal tree expansion is added after the vertical expansion. Each region H is itself divided further into smaller subregions. The subregion belonging to the candidate point that maximizes the acquisition function is vertically expanded in the next iteration of the optimization.

The hyperparameters that can be tuned for the optimization are the group sizes and the configuration of the acquisition functions ζ_{PI}, ζ_{EI} and η_{UCB}. Table I shows the combinations that are used in this work.

The optimization framework first selects an initial model configuration. The S-Parameters of that configuration are simulated with the physics-based via modeling and the FOM, which is the weighted power sum, is calculated. The optimization is working on the logarithmic problem, i.e. it tries to achieve the maximum of $\log(WSXTR)$ because it is advantageous to scale the output parameter range. The optimization framework repeats this sequence for a fixed number of iterations. The model that has achieved the best FOM so far is stored and compared with the current iteration.

IV. Single Via Model

The first model that is investigated is a single via surrounded by four ground vias (Fig. 4 (a)). A similar model was studied in [16]. All metal layers are GND layers (see Fig. 4 (b)). The objective function of the optimization is the weighted power sum of transmission (WPT). The parameters that are modified for this model are shown in Tab. II. In total seven parameters are included in the optimization the optimization. The antipad radius is calculated by adding the value k_{anti} to the via radius. Similarly, the pitch is calculated by adding k_{pitch} to $2 * r_{anti}$. This is necessary to remove the linear constraints of the parameters for the optimization.

Table II
PARAMETER RANGES OF THE LINK MODELS.

Parameter	Single Via	Via Array
$r_{via,sig}$	3-9 mil	3-9 mil
$r_{via,gnd}$	3-9 mil	3-9 mil
$r_{via,pwr}$	-	3-9 mil
$k_{anti,sig}$	2-6	2-6
$k_{anti,gnd}$	-	2-6
$k_{anti,pwr}$	-	2-6
k_{pitch}	30-50	30-50
t_{diel}	7-12 mil	7-12 mil
w_{sl}	-	4.3-4.5 mil
sig. layer	-	1-8
ε_r	3.6-4.5	3.6-4.5
$\tan\delta$	0-0.02	0-0.02

A. Optimization

The first optimization is for a bitrate of 15 Gbps. The BO finishes after 150 iterations, which has been found to be sufficient to achieve convergence. Table III shows the best parameters as well as the corresponding WPT for four different hyperparameter configurations that are defined in Table I. The convergence is shown in Fig. 5 (a). The group numbers do not impact the final result, however using a configuration of $\eta_{UCB} = 0.05$, $\zeta_{EI} = 0.1$, $\zeta_{PI} = 0.1$ results in a higher maximum.

The optimization is repeated for 25 and 35 Gbps with configurations C and D. The results are shown in Table IV and the convergence is shown in Fig. 6. Cases C and D result in an almost identical convergence for 25 Gbps and a small difference of the final value for 35 Gbps.

Another optimization used the Genetic Algorithm. The population size that is generated per generation is 50. For all bitrates the Genetic Algorithm converged after 4 generations. The convergence is shown in Fig. 5 and the results are shown in Table V. Overall, both the achieved maximum and the predicted best parameters are nearly the same as for the BO. One advantage of BO compared to GA is that it can be terminated after each iteration if a convergence is achieved. With GA, convergence is determined per generation.

B. Physical Interpretation

The predicted best parameters correlate well with the physical understanding of the via. All the parameters that are included in the optimization influence the impedance of the via. However, for the calculation of the WPT only the S_{21} parameter is of interest and the reflection parameter is excluded.

Fig. 7 shows the S-parameters of the single via for three different cases. The first case is the parameter configuration that

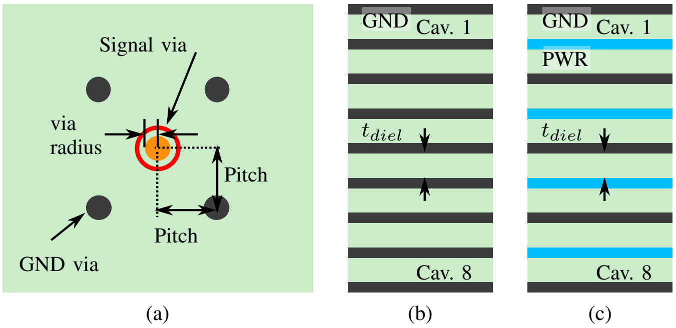


Fig. 4. Geometry of the single via link. (a) Top view of the single via model. The ports are at the top and bottom of the signal via. (b) The stack-up of the single via model. (c) The stack-up of the via array model.

Table III
BEST LINK PARAMETERS OF THE SINGLE VIA MODEL FOR 15 GBPS, PREDICTED WITH THE BAYESIAN OPTIMIZATION.

Parameter	A	B	C	D
$r_{via,sig}$	3.00	3.18	3.00	3.02
$r_{via,gnd}$	7.41	9.00	9.00	9.00
$r_{anti,sig}$	5.24	6.18	5.25	6.02
$pitch$	40.47	42.36	40.50	42.05
t_{diel}	7.08	9.58	8.25	8.25
ε_r	3.50	3.51	3.50	3.51
$\tan\delta$	0.00	0.00	0.00	0.00
WPT	6337.90	6341.20	6349.01	6346.98

generates the highest WPT for 15 Gbps (with configuration C). The other two are the first two settings that are generated during the optimization process and generate a lower WPT. Up to approximately 40 GHz it can clearly be seen that the transmission of the best case scenario is considerably higher than for the other two cases. Similarly, the reflection is lower. This explains why the best case is favorable at least for smaller bitrates because in that case the signal energy is concentrated in the lower frequency regions.

The behavior of a single via was previously studied in [17]. GND vias in close proximity to the signal via are critical because they confine the field around the signal via and provide a defined return current path. A change in ground via radius also affects the impedance but the impact is less than the ground via distance. Increasing the dielectric height also increases the via impedance. Changing the via radius and antipad radius changes the via capacitance. A lower capacitance value increases the via impedance.

If the via is designed manually, it would be useful to select the smallest distance between ground and signal via first. Similarly, the dielectric loss should be as small as possible, as would have been the dielectric height. Afterwards the via parameters (via and antipad radius as well as ground via radius) can be tuned.

V. VIA ARRAY MODEL

The via array model is shown in Fig. 3. Ports are either placed on the vias (red circles) or at the end of the striplines (blue circles). The stack-up is shown in Fig. 4(c). The S-parameters are simulated with the physics-based via modeling. The weighted power sum of crosstalk is calculated for the victim port 16 with aggressor ports 11,13,17,19. The weighted power sum of transmission is calculated for the transmission between port 16 and 15. The optimization goal was to improve the WSXTR. In total 12 parameters are considered for the optimization. Their range is given in Table II.

Table IV
BEST LINK PARAMETERS OF THE SINGLE VIA MODEL FOR 25 AND 35 GBPS, PREDICTED WITH THE BAYESIAN OPTIMIZATION.

Parameter	25 Gbps C	25 Gbps D	35 Gbps C	35 Gbps D
$r_{via,sig}$	3.00	3.00	3.02	3.01
$r_{via,gnd}$	7.50	7.50	8.99	9.00
$r_{anti,sig}$	5.06	5.75	5.41	5.47
$pitch$	40.12	41.50	40.91	40.96
t_{diel}	8.25	7.00	7.31	7.00
ε_r	3.50	3.62	3.50	3.50
$\tan\delta$	0.00	0.00	0.01	0.00
WPT	7894.41	7892.57	9524.31	9544.83

Table V
BEST LINK PARAMETERS OF THE SINGLE VIA MODEL, PREDICTED WITH THE GENETIC ALGORITHM.

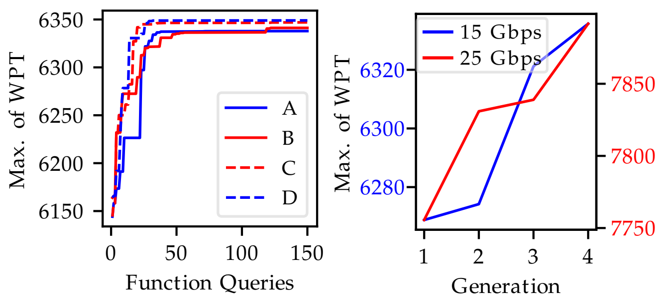
Parameter	15 Gbps	25 Gbps	35 Gbps
$r_{via,sig}$	3.00	3.15	3.00
$r_{via,gnd}$	8.05	8.63	7.78
$r_{anti,sig}$	5.00	5.15	5.22
$pitch$	40.00	40.30	45.97
t_{diel}	7.00	8.99	7.00
ε_r	3.50	3.50	3.50
$\tan\delta$	0.01	0.01	0.01
WPT	6335.68	7891.58	9398.80

A. Optimization

At first, the link is optimized with the BO for a bitrate of 15 Gbps. The optimization terminates after 150 iterations. Different configurations (see Tab. I) of the optimization algorithm are tested. The convergence is shown in Fig. 8 (a). The corresponding parameters that are predicted as the optimal choice are given in Tab. VI. It also presents the maximum WSXTR that is achieved for each configuration. The final value of the WSXTR is nearly the same for all hyperparameter configurations with the exception of case A, where the value is significantly smaller.

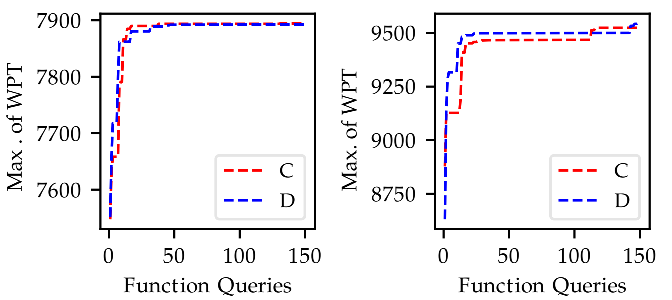
The results for 25 and 35 Gbps are shown in Fig. 9. The optimization used the hyperparameter cases A and C. For both 25 and 35 Gbps, the difference between A and C is not as big as for 15 Gbps. The maximum value that is achieved is considerably smaller than for 15 Gbps. Table VII gives the best parameter configurations that are predicted from the optimization.

The BO was again compared with a Genetic Algorithm. The population size per generation is 50 and the algorithm converged after 4 generations. The convergence for 15 and 25 Gbps is shown in Fig. 8(b) and Table VIII shows the resulting parameters for 15 and 25 Gbps. The predicted best values are not identical to the results from the BO, however



(a) (b)

Fig. 5. Optimization of the single via model. (a) Convergence of the Bayesian Optimization for the single via for 15 Gbps. The legend refers to Tab. I. (b) Convergence of the Genetic Algorithm for 15 and 25 Gbps. The blue y-axis on the left refers to 15 Gbps. The red y-axis on the right refers to 25 Gbps.



(a) (b)

Fig. 6. Convergence of the Bayesian Optimization for the single via for 25 Gbps and 35 Gbps. The legend refers to Tab. I. (a) 25 Gbps. (b) 35 Gbps.

they are in the same order of magnitude. For 15 Gbps a higher final value can be achieved with the BO. However, for 25 Gbps the Genetic Algorithm yields a better value than the BO.

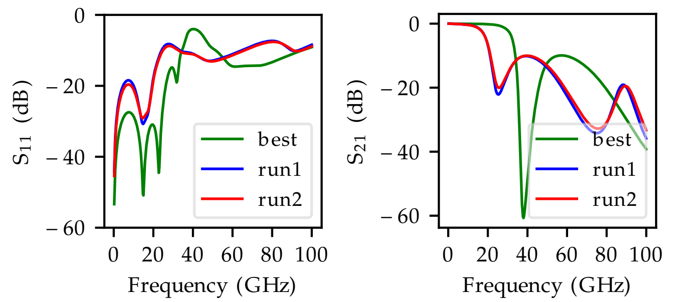
Table VI
BEST LINK PARAMETERS OF THE VIA ARRAY MODEL FOR 15 GBPS, PREDICTED WITH THE BAYESIAN OPTIMIZATION.

Parameter	A	B	C	D
$r_{via,sig}$	8.98	7.50	9.00	4.31
$r_{via,gnd}$	8.99	8.81	9.00	8.99
$r_{via,pwr}$	8.81	8.98	8.91	4.31
$r_{anti,sig}$	14.20	10.50	14.37	6.33
$r_{anti,gnd}$	14.36	14.81	12.81	13.98
$r_{anti,pwr}$	11.63	12.73	14.41	10.30
$pitch$	73.57	62.27	59.44	77.57
t_{diel}	11.43	7.01	7.31	7.14
ε_r	4.49	3.63	3.53	4.49
$\tan\delta$	0.020	0.014	0.010	0.020
w_{sl}	4.33	4.40	4.47	4.33
sig. layer	1	1	1	1
WSXTR	163.22	230.75	243.59	230.15

B. Physical Interpretation

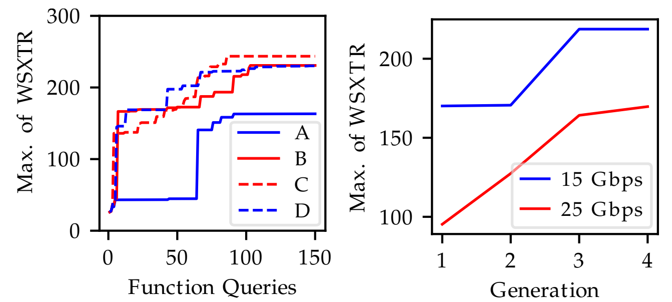
Fig. 10 shows the differential transmission and one FEXT parameter for the via array model for three cases. One is the case that generated the highest WSXTR for 15 Gbps with hyperparameter configuration case C. The other two are the first two samples generated during the optimization. The best case has both a significantly higher transmission and a lower crosstalk level.

The dependencies of WPSXT and WPT were previously studied in [6], [12] for a via array and an array to array link. For the single via array the via pitch should be small so that a good field confinement from the GND vias can be achieved. For a link that also included striplines the increased crosstalk in the stripline due to the tighter spacing part partially counteracts this effect. There is an optimum in the center of the parameter range. A lower dielectric height was also found to increase the WSXTR. The dielectric loss simultaneously reduces the transmission and the far-end crosstalk. In the array model presented in this work, the striplines are very short so the adverse effect of the loss on the transmission is not as prominent. This explains why the optimization predicts a medium to high loss tangent. In [12] it was shown that for a similar link a small dielectric height and a large via radius are favorable to achieve a large WSXTR. This correlates with the optimization results.



(a) (b)

Fig. 7. S-parameters of the single via model for 15 Gbps for the highest predicted value (with configuration C) and the S-parameter of the first two iterations of the optimization. (a) S_{11}. (b) S_{21}.

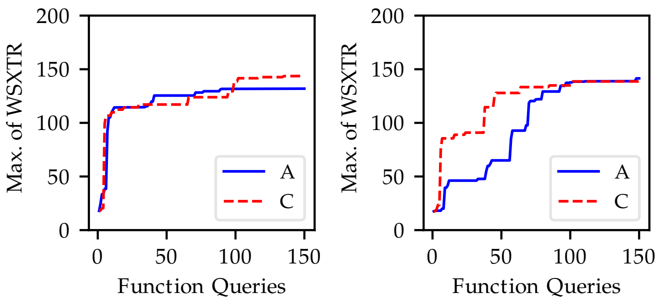


(a) (b)

Fig. 8. Optimization results for the via array model. (a) Convergence of the Bayesian Optimization for 15 Gbps. The legend refers to Tab. I. (b) Convergence of the Genetic Algorithm for 15 and 25 Gbps.

VI. CONCLUSIONS

Bayesian Optimization can be an efficient method for the design of high-speed links. For a single via link the results are consistent with the Genetic Algorithm and the physically derived design. For the more complex via array model a larger dependency on the hyperparameters of the Bayesian Optimization can be observed. The predicted design parameters correlate with results from previous studies of similar links.



(a) (b)

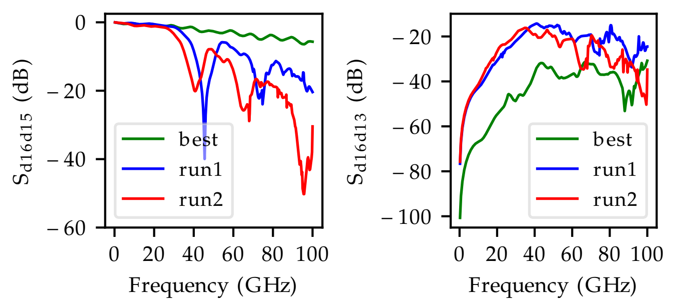
Fig. 9. Convergence of the Bayesian Optimization for the via array for 25 Gbps and 35 Gbps. The legend refers to Tab. I. (a) 25 Gbps. (b) 35 Gbps.

Table VII
BEST PARAMETERS FROM THE BAYESIAN OPTIMIZATION FOR 25 AND 35 GBPS.

Parameter	25 Gbps A	25 Gbps C	35 Gbps A	35 Gbps C
$r_{via,sig}$	6.70	8.63	3.28	8.91
$r_{via,gnd}$	7.49	8.81	3.00	6.00
$r_{via,pwr}$	6.38	8.27	8.95	8.91
$r_{anti,sig}$	10.94	14.19	7.28	11.41
$r_{anti,gnd}$	9.50	12.06	5.75	8.45
$r_{anti,pwr}$	11.37	13.88	14.89	14.41
$pitch$	52.74	59.96	69.51	78.77
t_{diel}	10.99	7.00	7.04	7.00
ε_r	3.62	3.75	4.50	4.06
$\tan\delta$	0.02	0.01	0.02	0.01
w_{sl}	4.32	4.35	4.31	4.40
sig. layer	1	1	1	1
WSXTR	131.90	143.66	141.46	138.60

Table VIII
BEST LINK PARAMETERS OF THE VIA ARRAY MODEL, PREDICTED WITH THE GENETIC ALGORITHM

Parameter	15 Gbps	25 Gbps
$r_{via,sig}$	4.15	7.51
$r_{via,gnd}$	8.09	8.49
$r_{via,pwr}$	8.64	8.67
$r_{anti,sig}$	8.59	11.12
$r_{anti,gnd}$	14.04	12.68
$r_{anti,pwr}$	13.22	10.67
$pitch$	74.95	55.35
t_{diel}	7.62	7.00
ε_r	4.20	3.67
$\tan\delta$	0.02	0.01
w_{sl}	4.40	4.45
sig. layer	1	1
WSXTR	218.72	169.71



(a) (b)

Fig. 10. S-parameters of the via array model for the highest predicted value for 15 Gbps for configuration C and two randomly chosen S-parameter sets. (a) Transmission. (b) FEXT.

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