3 Physical Background

3.1 S-Matrix Calculus

To implement the desired algorithm we need to be able to calculate the optical behavior of stacked meta surfaces. The mathematical framework we will use is called Scatter Matrix Calculus and this section will give some insight into its physical origin and how to use it. We will start with the Maxwell Equations in matter.

Maxwell Equations

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t) \tag{3.1}$$

$$\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho_{\text{ext}}(\mathbf{r},t) \tag{3.2}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t) + \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) \tag{3.3}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0 \tag{3.4}$$

The four involved fields are: $\mathbf{E}$...electric field, $\mathbf{B}$...magnetic flux density, $\mathbf{D}$...electric flux density and $\mathbf{H}$...magnetic field and the sources are the external charges ρ_{ext} and the macroscopic currents j. All the material properties are captured by the $\mathbf{D}$ and $\mathbf{H}$ fields which are defined as:

$$\begin{aligned}\mathbf{D}(\mathbf{r},t) &= \varepsilon_0\mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t)\\ \mathbf{H}(\mathbf{r},t) &= \frac{1}{\mu_0}[\mathbf{B}(\mathbf{r},t) - \mathbf{M}(\mathbf{r},t)]\end{aligned} \tag{3.5}$$

Where $\mathbf{P}$ is the dielectric polarization and $\mathbf{M}$ is the magnetic polarization. One can read equation (3.5) in the following way: When the electric field $\mathbf{E}$ interacts with matter it exerts a force on all its charges and displaces them by a small amount. The separation of charges results in a counter field $\mathbf{P}$ and the total field $\mathbf{D}$ is now a superposition of $\mathbf{E}$ and $\mathbf{P}$. This set of equations describes the whole electromagnetic spectrum, in this work however we are only interested in visible (VIS) and near infrared (NIR) light where we can make some simplifications. Generally in optics materials are non-magnetizable so $\mathbf{M} = 0$ and there are no free charges $\rho_{\text{ext}} = 0$. Inserting these assumptions into the maxwell equation gives:

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\mu_0\frac{\partial}{\partial t}\mathbf{H}(\mathbf{r},t) \tag{3.6}$$

$$\varepsilon_0\nabla \cdot \mathbf{E}(\mathbf{r},t) = -\nabla \cdot \mathbf{P}(\mathbf{r},t) \tag{3.7}$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t) + \frac{\partial}{\partial t}\mathbf{P}(\mathbf{r},t) + \varepsilon_0\frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) \tag{3.8}$$

$$\nabla \cdot \mathbf{H}(\mathbf{r},t) = 0 \tag{3.9}$$

Light in Vacuum

Now we can derive the famous wave equation by considering $\nabla\times$ (3.6):

$$\begin{aligned}&\nabla \times \left[\nabla \times \mathbf{E}\right] = \nabla \times \left[-\mu_0\frac{\partial}{\partial t}\mathbf{H}\right]\\ \iff\quad &\nabla(\nabla \cdot \mathbf{E}) - \Delta\mathbf{E} = -\mu_0\frac{\partial}{\partial t}\nabla \times \mathbf{H} \quad \Big| \text{ subs. (3.8) and (3.7)}\\ \iff\quad &\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E} - \Delta\mathbf{E} = -\mu_0\frac{\partial}{\partial t}\mathbf{j} - \mu_0\frac{\partial^2}{\partial t^2}\mathbf{P} + \frac{1}{\varepsilon_0}\nabla(\nabla \cdot \mathbf{P})\end{aligned} \tag{3.10}$$

In vacuum ($\mathbf{P} = 0$ and $\mathbf{j} = 0$) the right side of this equation vanishes and we are left with $\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E} - \Delta\mathbf{E} = 0$ which is solved by the plane wave $\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{kr}-\omega t)}$ where $\frac{\omega}{k} = c$. This describes the propagation of light through empty space: a sinusoidal oscillation in time and space along the $\mathbf{k}$ direction where $\mathbf{E}$, $\mathbf{B}$ and $\mathbf{k}$ are all perpendicular to each other. **1.this needs details 2.show figure?**

Light in homogeneous, isotropic materials

The next question we can answer is how light propagates through a homogeneous and isotropic material. For us, the dielectric polarization is some linear function of the electric field so $\mathbf{P}(\mathbf{r},t) = \hat{\chi}(\omega,\mathbf{r})\mathbf{E}(\mathbf{r},t)$. An isotropic material behaves the same for all orientations of $\mathbf{E}$ that means $\hat{\chi}(\omega,\mathbf{r})$ becomes a scalar function $\chi(\omega,\mathbf{r})$. If the material is additionally homogeneous, that is the same everywhere independent of $\mathbf{r}$, then $\boldsymbol{\nabla}\chi(\omega,\mathbf{r}) = 0$. With equation (3.7) this gives us $\boldsymbol{\nabla}\cdot\mathbf{P} = 0$ and the wave equation simplifies to:

$$\begin{aligned} \frac{\varepsilon}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E} - \Delta\mathbf{E} &= 0 \\ \text{where} \quad \varepsilon\,\mathbf{E} := (1+\chi)\mathbf{E} &= \mathbf{E} + \mathbf{P} \end{aligned} \tag{3.11}$$

That means light behaves in these materials exactly as it would in vacuum we only have to account for a decreased speed of light $c' = \frac{c}{\sqrt{\varepsilon}} =: \frac{c}{n}$ with the refractive index n. This is equivalent to a decreased wavelength $\lambda' =: \frac{\lambda}{n}$ or an increased wave vector $k' = \frac{2\pi}{\lambda'} = n\,k$. A complex valued $n := \eta + i\kappa$ even captures the possibility of an exponentially decaying field:

$$\mathbf{E} = \mathbf{E}_0 e^{i(n\mathbf{kr}-\omega t)} = \mathbf{E}_0 \underbrace{e^{-\kappa\mathbf{kr}}}_{\text{decay}} \underbrace{e^{i(\eta\mathbf{kr}-\omega t)}}_{\text{oscillation}} \tag{3.12}$$

Interfaces

The meta surface stacks we want to understand are obviously not one homogeneous material. Rather they contain many interfaces between different materials and we can again use the maxwell equations to predict how light will behave at such an interface.

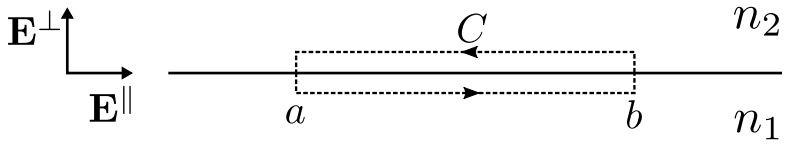

Figure 1: An interface of two materials with different refractive indices n_1 and n_2 and a closed contour C which is tangent to the interface between the points a and b.

Let us consider a closed contour C around an interface as seen in Figure 1 and integrate the first maxwell equation (3.6) over the surface A enclosed by that contour:

$$\begin{aligned} \int_A \boldsymbol{\nabla}\times\mathbf{E}(\mathbf{r},t)\,\mathrm{d}\mathbf{A} &= -\mu_0\frac{\partial}{\partial t}\int_A \mathbf{H}(\mathbf{r},t)\mathrm{d}\mathbf{A} \\ \overset{\text{stokes}}{\Longleftrightarrow} \qquad \int_{C=\partial A} \mathbf{E}(\mathbf{r},t)\mathrm{d}\mathbf{r} &= -\mu_0\frac{\partial}{\partial t}\int_A \mathbf{H}(\mathbf{r},t)\mathrm{d}\mathbf{A} \end{aligned} \tag{3.13}$$

But now we can bring the contour infinitely close to the interface and thus reduce the right hand side of the equation, the total magnetic flux, through the surface, to zero. That leaves us with:

$$\begin{aligned} \int_a^b \mathbf{E}_1\,\mathrm{d}\mathbf{r} \;+ \int_b^a \mathbf{E}_2\,\mathrm{d}\mathbf{r} &= 0 \\ \Longleftrightarrow \qquad \int_a^b \mathbf{E}_1\,\mathrm{d}\mathbf{r} &= \int_a^b \mathbf{E}_2\,\mathrm{d}\mathbf{r} \end{aligned} \tag{3.14}$$

Because a and b were chosen arbitrarily that means that the transverse field components along the path need to be continuous so $\mathbf{E}_1^{\parallel} = \mathbf{E}_2^{\parallel}$. The analog expression $\mathbf{H}_1^{\parallel} = \mathbf{H}_2^{\parallel}$ can be shown by starting with the third maxwell equation (3.8) instead. We can now use these continuity conditions to learn more about the behavior of light at these interfaces.

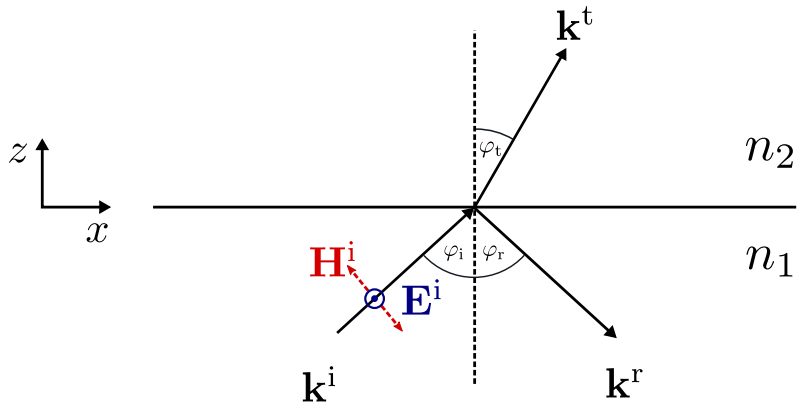

Figure 2: Interface between two materials of different refractive indices n_1 and n_2. The incident light has a wave vector $\mathbf{k}^{\mathrm{i}}$ and is partially transmitted and partially reflected. The fields are shown in transverse electric (TE) polarization where $\mathbf{H}$ is in the x-z plane and $\mathbf{E}$ occilates in the y direction.

Let us consider the same interface from before and have an incident field $\mathbf{E}^{\mathrm{i}}$ interact with it. From figure 2 we can see:

$$\mathbf{k}^{\mathrm{i}} = k_0 n_1 \begin{pmatrix} -\sin\varphi_{\mathrm{i}} \\ 0 \\ -\cos\varphi_{\mathrm{i}} \end{pmatrix}, \quad \mathbf{k}^{\mathrm{r}} = k_0 n_1 \begin{pmatrix} \sin\varphi_{\mathrm{r}} \\ 0 \\ -\cos\varphi_{\mathrm{r}} \end{pmatrix}, \quad \mathbf{k}^{\mathrm{t}} = k_0 n_2 \begin{pmatrix} \sin\varphi_{\mathrm{t}} \\ 0 \\ \cos\varphi_{\mathrm{t}} \end{pmatrix} \tag{3.15}$$

Now we can decompose the electric field into two orthogonal polarizations. One component were $\mathbf{E} = E\,\vec{\mathbf{e}_{\mathbf{y}}}$ called transverse electric (TE) as shown in figure 2 and its orthogonal component where $\mathbf{H} = H\,\vec{\mathbf{e}_{\mathbf{y}}}$ called transverse magnetic (TM). If we apply the continuity condition from before to the TE component we get $\mathbf{E}_1 = \mathbf{E}_2$ at $z = 0$:

$$\begin{aligned} \mathbf{E}^{\mathrm{i}} + \mathbf{E}^{\mathrm{r}} &= \mathbf{E}^{\mathrm{t}} \\ E^{\mathrm{i}} e^{i(k_x^{\mathrm{i}} x)} + E^{\mathrm{r}} e^{i(k_x^{\mathrm{r}} x)} &= E^{\mathrm{t}} e^{i(k_x^{\mathrm{t}} x)} \end{aligned} \tag{3.16}$$

This is only possible for all x if:

$$E^{\mathrm{i}} + E^{\mathrm{r}} = E^{\mathrm{t}} \quad \text{and} \quad k_x^{\mathrm{i}} = k_x^{\mathrm{r}} = k_x^{\mathrm{t}} \tag{3.17}$$

Two basic laws of optics lie in this relation: The law of reflection

$$k_x^{\mathrm{i}} = k_x^{\mathrm{r}} \quad \Rightarrow \quad k_0 n_1 \sin\varphi_i = k_0 n_1 \sin\varphi_r \quad \Rightarrow \quad \varphi_i = \varphi_r := \varphi_1 \tag{3.18}$$

and the Snells law of refraction

$$k_x^{\mathrm{i}} = k_x^{\mathrm{t}} \quad \Rightarrow \quad k_0 n_1 \sin\varphi_i = k_0 n_2 \sin\varphi_t \quad \Rightarrow \quad n_1 \sin\varphi_i = n_2 \sin\varphi_t \tag{3.19}$$

Fresnel Equations

To fully describe an interface we also need know the fraction of the transmitted $t := E^t/E^i$ and the reflected $r := E^r/E^i$ fields. Again using the TE polarization we have an orientation of fields were $\mathbf{E} = E\,\vec{\mathbf{e}}_y$ and $\mathbf{H}$ is contained perpendicular to $\mathbf{E}$ in the x-z plane:

$$\mathbf{H}^{\mathrm{i}} = H^{\mathrm{i}} \begin{pmatrix} -\cos\varphi_{\mathrm{i}} \\ 0 \\ -\sin\varphi_{\mathrm{i}} \end{pmatrix}, \quad \mathbf{H}^{\mathrm{r}} = H^{\mathrm{r}} \begin{pmatrix} \cos\varphi_{\mathrm{r}} \\ 0 \\ \sin\varphi_{\mathrm{r}} \end{pmatrix}, \quad \mathbf{H}^{\mathrm{t}} = H^{\mathrm{t}} \begin{pmatrix} -\cos\varphi_{\mathrm{t}} \\ 0 \\ \sin\varphi_{\mathrm{t}} \end{pmatrix} \tag{3.20}$$

The H_x component is tangent to the interface so it also needs to be continuous across the boundary:

$$\begin{aligned} & H_x^{\mathrm{i}} + H_x^{\mathrm{r}} = H_x^{\mathrm{t}} \\ \Longleftrightarrow \qquad & H^{\mathrm{i}} \cos\varphi_1 - H^{\mathrm{r}} \cos\varphi_1 = H^{\mathrm{t}} \cos\varphi_2 \end{aligned} \tag{3.21}$$

Maxwells first equation (3.6) allows us connect the magnitudes of $\mathbf{H}$ and $\mathbf{E}$ via the refractive index $H \sim n\,E$. This changes (3.21) to:

$$n_1\,E^{\mathrm{i}}\cos\varphi_1 - n_1\,E^{\mathrm{r}}\cos\varphi_1 = n_2\,E^{\mathrm{t}}\cos\varphi_2 \tag{3.22}$$

Substituting E^{r} or E^{i} with (3.17) and rearranging we get:

$$t = \frac{2n_1\cos\varphi_1}{n_1\cos\varphi_1 + n_2\cos\varphi_2} \quad \text{and} \quad r = \frac{n_1\cos\varphi_1 - n_2\cos\varphi_2}{n_1\cos\varphi_1 + n_2\cos\varphi_2} \tag{3.23}$$

These are called the Fresnel equations for the TE component. The TM component can be treated analogous which yields:

$$t = \frac{2n_1\cos\varphi_1}{n_2\cos\varphi_1 + n_1\cos\varphi_2} \quad \text{and} \quad r = \frac{n_2\cos\varphi_1 - n_1\cos\varphi_2}{n_2\cos\varphi_1 + n_1\cos\varphi_2} \tag{3.24}$$

For perpendicular incident light at $\varphi = 90°$ these should describe the same situation as we can no longer differentiate between TE and TM components and indeed for this angle they are equivalent if we consider that the TE factors describe the electric field and the TM factors describe the magnetic field. The TE factors become:

$$t = \frac{2n_1}{n_1 + n_2} \quad \text{and} \quad r = \frac{n_1 - n_2}{n_1 + n_2} \tag{3.25}$$

Stacking

We can take this one step further by including interfaces which have incident light from both sides. Let $\mathbf{E}_{\mathrm{out}}$ be the light coming out of the interface and $\mathbf{E}_{\mathrm{in}}$ be the light going into the interface as seen in figure 3:

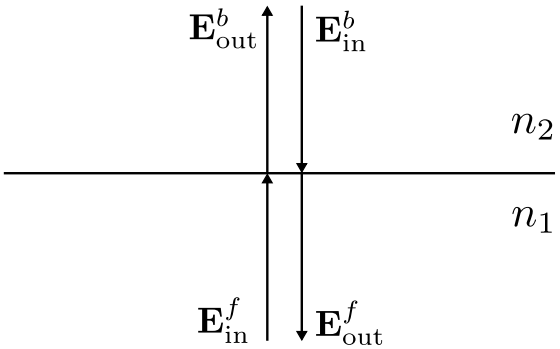

Figure 3: Interface between two materials of different refractive indices n_1 and n_2 were incident light is coming from the front and the back.

Using the factors from the Fresnel equations we get:

$$E^b_{\mathrm{out}} = E^f_{\mathrm{in}}\,t^f + E^b_{\mathrm{in}}\,r^b \quad \text{and} \quad E^f_{\mathrm{out}} = E^b_{\mathrm{in}}\,t^b + E^f_{\mathrm{in}}\,r^f \tag{3.26}$$

This can concisely be expressed using matrices and vectors:

$$\begin{pmatrix} E^f_{\mathrm{out}} \\ E^b_{\mathrm{out}} \end{pmatrix} = \underbrace{\begin{pmatrix} t^f & r^b \\ r^f & t^b \end{pmatrix}}_{=:\hat{S}} \begin{pmatrix} E^f_{\mathrm{in}} \\ E^b_{\mathrm{in}} \end{pmatrix} \tag{3.27}$$

We call these matrices mapping field-in to field-out S-matrices. They can be used to describe more than just an interface. As shown in the paragraph Light in materials when light propagates through homogeneous isotropic material just the phase changes by a factor of e^{ik_0nd} where d is the distance traveled. We can express this by allowing complex valued t and r:

$$\hat{S}_{n,d} = \begin{pmatrix} e^{ik_0 nd} & 0 \\ 0 & e^{ik_0 nd} \end{pmatrix} \tag{3.28}$$

Analogue the S-matrix for an interface from n_1 to n_2 is:

$$\hat{S}_{n_1,n_2} = \begin{pmatrix} \frac{2n_1}{n_1+n_2} & \frac{n_2-n_1}{n_1+n_2} \\ \frac{n_1-n_2}{n_1+n_2} & \frac{2n_1}{n_1+n_2} \end{pmatrix} \tag{3.29}$$

Say we have a stack of different homogeneous isotropic materials. We are now are now able to write down an S-matrix for every part of the stack that is every interface and every propagation between interfaces as seen in figure 4, but we cannot predict the behavior of the stack as a whole:

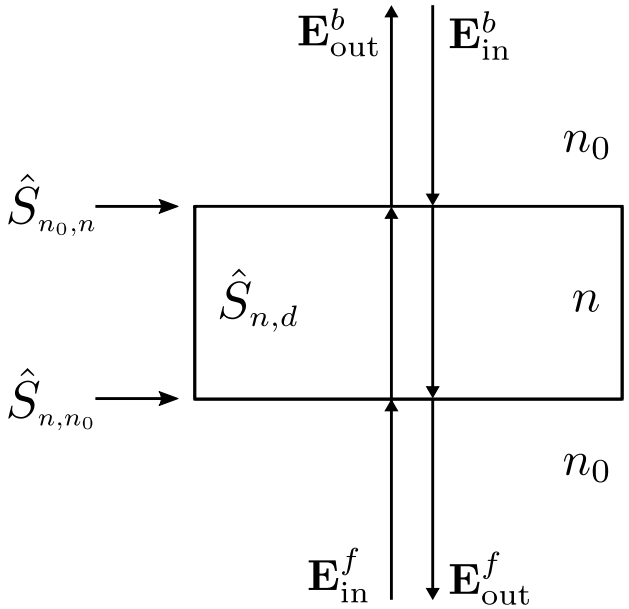

Figure 4: A slab of one homogeneous isotropic material with thickness d in air (n_0). This setup is described by two interface and one propergation S-matrices.

The combined S-matrix $\hat{S}$ consisting of $\hat{S}_1$ and $\hat{S}_2$ cannot be obtained by simply using the matrix product. The result would be:

$$\hat{S}_1\,\hat{S}_2 = \begin{pmatrix} t_1^f\,t_2^f + r_1^b\,r_2^f & t_1^f\,r_2^b + r_1^b\,t_2^b \\ r_1^f\,t_2^f + t_1^b\,r_2^f & r_1^f\,r_2^b + t_1^b\,t_2^b \end{pmatrix} \neq \begin{pmatrix} t^f & r^b \\ r^f & t^b \end{pmatrix} = \hat{S} \tag{3.30}$$

and this would imply that the transmission from the front t^f increases when the internal reflections of the system r_1^b and r_2^f increase which is the opposite of the behavior we expect. Redheffer [**?**] studied these kind of systems in the 60s and found an operator $\star$ which yields the combined S-matrix:

$$\hat{S}_1 \star \hat{S}_2 := \begin{pmatrix} t_2^f(1-r_1^b r_2^f)^{-1}t_1^f & r_2^b + t_2^f r_1^b(1-r_2^f r_1^b)^{-1}t_2^b \\ r_1^f + t_1^b r_2^f(1-r_1^b r_2^f)^{-1}t_1^f & t_1^b(1-r_2^f r_1^b)^{-1}t_2^b \end{pmatrix} \tag{3.31}$$

For this operation to produce physically valid results certain condition have to be met. We will discuss these in detail in the paragraph Conditions of section 3.2. Applied to the example of figure 4 that gives:

$$\hat{S} = \hat{S}_{n_0,n} \star \hat{S}_{n,d} \star \hat{S}_{n,n_0} \tag{3.32}$$

Polarization

Up to this point we are dealing with vectors of the form $\begin{pmatrix} E_{\text{in}}^f \\ E_{\text{in}}^b \end{pmatrix}$ where E_{in}^f and E_{in}^b are scalar properties. That means we can only describe linear polarized light in one direction. The last generalization we want to make is to extend this formalism to all polarizations. As shown in the paragraph Light in materials a planar light wave propagating along the z axis through a homogeneous isotropic material can be described as:

$$\mathbf{E} = \begin{pmatrix} E_x e^{i(kz-\omega t+\varphi_x)} \\ E_y e^{i(kz-\omega t+\varphi_y)} \\ 0 \end{pmatrix} = \left(E_x\, e^{i\varphi_x}\, \vec{\mathbf{e_x}} + E_y\, e^{i\varphi_y}\, \vec{\mathbf{e_y}}\right) e^{i(kz-\omega t)} \tag{3.33}$$

the waves polarization is determined by the scaling factors of $\vec{\mathbf{e_x}}$ and $\vec{\mathbf{e_y}}$ and can be expressed as a *Jones Vector* $\mathbf{j} \in \mathbb{C}^2$.

$$\mathbf{j} = \frac{1}{\sqrt{E_x^2 + E_y^2}} \begin{pmatrix} E_x \\ E_y\, e^{i\delta} \end{pmatrix} \quad \text{with} \quad \delta := \varphi_y - \varphi_x \tag{3.34}$$

Now all linear operations on the polarization are matrices $\hat{M} \in \mathbb{C}^{2\times 2}$. That means all passive components have a corresponding matrix. A couple examples for components in horizontal position:

$$\begin{aligned} \text{polarizer:} \quad & \hat{M} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ \lambda/4 \text{ plate:} \quad & \hat{M} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} e^{-\frac{i\pi}{4}} \\ \lambda/2 \text{ plate:} \quad & \hat{M} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \end{aligned} \tag{3.35}$$

We can now generalize the S-matrix Calculus simply by allowing proper Jones matrices in place of the Fresnel factors: $t \to \hat{T}$ and $r \to \hat{R}$. The star product of two S-matrices becomes:

$$\hat{S}_1 \star \hat{S}_2 = \begin{pmatrix} \hat{T}_1^f & \hat{R}_1^b \\ \hat{R}_1^f & \hat{T}_1^b \end{pmatrix} \star \begin{pmatrix} \hat{T}_2^f & \hat{R}_2^b \\ \hat{R}_2^f & \hat{T}_2^b \end{pmatrix} = \begin{pmatrix} \hat{T}_2^f (\mathbb{1} - \hat{R}_1^b \hat{R}_2^f)^{-1} \hat{T}_1^f & \hat{R}_2^b + \hat{T}_2^f \hat{R}_1^b (\mathbb{1} - \hat{R}_2^f \hat{R}_1^b)^{-1} \hat{T}_2^b \\ \hat{R}_1^f + \hat{T}_1^b \hat{R}_2^f (\mathbb{1} - \hat{R}_1^b \hat{R}_2^f)^{-1} \hat{T}_1^f & \hat{T}_1^b (\mathbb{1} - \hat{R}_2^f \hat{R}_1^b)^{-1} \hat{T}_2^b \end{pmatrix} \tag{3.36}$$

So the general S-matrix is $\hat{S} \in \mathbb{C}^{4\times 4}$ and consist of four separate Jones matrices.

3.2 SASA

The S-matrix calculus enables us to calculate the optical behavior of a stack if we know the optical behavior of all its layers in the form of their S-matrices. In section 3.1 we derived the S-matrices of propagation through and interfaces between homogeneous isotropic materials. This calculation is based on the Fresnel equations and is analytic. We cannot however calculate the S-matrix of a meta surface analytically. This results in a "Semi Analytic" Stacking Algorithm where the S-matrices of the meta surfaces need to be provided but the remaining S-matrices can be calculated based on the stack parameters.

3.insert figure of two layer stack

Importantly symmetry operations like rotation and mirroring can be applied directly to Jones matrices. For example let $\hat{M}$ be the Jones matrix of an optical component then the Jones matrix of the rotated component $\hat{M}_\varphi$ is calculated as:

$$\hat{M}_\varphi = \hat{\Theta}(-\varphi)\,\hat{M}\,\hat{\Theta}(\varphi) \quad \text{where} \quad \hat{\Theta}(\varphi) = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \tag{3.37}$$

On this basis we can rotate S-matrices in a similar manner:

$$\hat{S}_\varphi = \begin{pmatrix} \hat{\Theta}(-\varphi)\hat{T}^f\hat{\Theta}(\varphi) & \hat{\Theta}(-\varphi)\hat{R}^b\hat{\Theta}(\varphi) \\ \hat{\Theta}(-\varphi)\hat{R}^f\hat{\Theta}(\varphi) & \hat{\Theta}(-\varphi)\hat{T}^b\hat{\Theta}(\varphi) \end{pmatrix} \tag{3.38}$$

Flipping and mirroring of S-matrices is done analogously.With this all mathematical operations are well defined and we can write down SASA in pseudo code:

Input: Stack = [Layer 1, Layer 2, ...]
Output: Stack S-matrix
S-mats = [ ]
for $i = 0$; $i <$ len(Stack); $i = i + 1$; **do**
  if *Stack*[i] **is** *meta surface* **then**
    add layer $\hat{S}$ to S-mats
  else
    calculate propagation S-matrix $\hat{S}_{n_i,d_i}$
    add $\hat{S}_{n_i,d_i}$ to S-mats
  end
  calculate interface S-matrix $\hat{S}_{n_i,n_{i+1}}$
  add $\hat{S}_{n_i,n_{i+1}}$ to S-mats
end
$\hat{S} = \mathbb{1}$
for $i = 0$; $i <$ len(*S-mats*); $i = i + 1$; **do**
  $\hat{S} = \hat{S} \star S\text{-mats}[i]$
end
return $\hat{S}$

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Conditions

For this algorithm to produce physical valid output some conditions need to be met

3.3 Neural Networks

Artificial Neural Networks (ANN's or short NN's) are a kind of data structure inspired by the biological neurons found in nature. They can be used to find a wide range of input output relations. One classic example is mapping pictures of hand written digits to the actual digits. Rather than explicitly programmed, NN's are trained on a dataset (X, Y) of correct input output pairs.

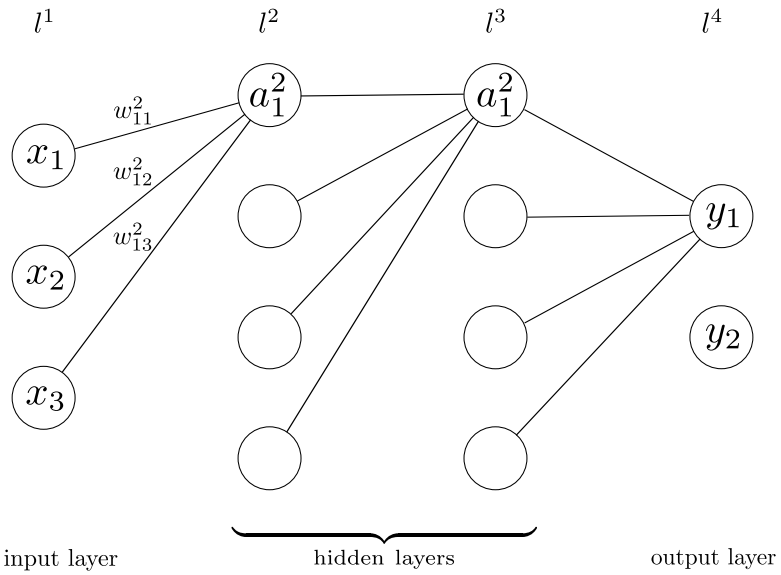


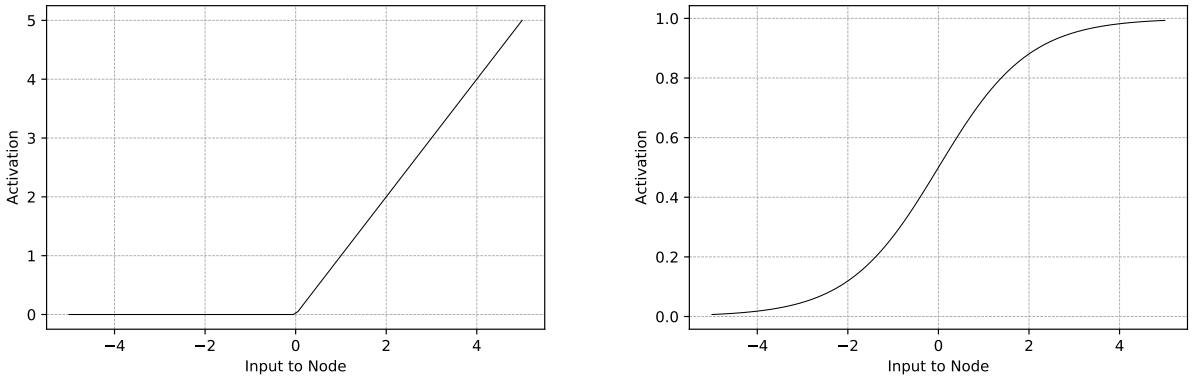
Figure 5: The most simple kind of NN is called densely connected or multilayer perceptron. For clarity only connections to the top most node of each layer are shown.

Multilayer Perceptron This kind of classic NN consist of single nodes or neurons which are organized into layers. The terms node and neuron can be used interchangeably. Every node is connected to all the nodes of the previous and the next layer. For this reason the network is called dense or densely connected. Each node holds a value called activation a where the activation to the first layer is the input to the network, here: (x_1, x_2, x_3). The nodes are connected by weights w which specify how much one node should influence the next and every node has a bias b to control at what total input activation the node itself should become active. To calculate the activation of a node one has to multiply all the activations of the previous layer with their respective weights w, add the bias b and finally apply a non-linear activation function σ as seen in Figure 6. To describe this process mathematically we are going to use the usual index notation where superscripts specify the layer and subscripts the node. So a^2_1 is the activation of the first node in the second layer. To characterize a weight two subscripts are needed for the end and beginning of the connection. For the example in figure 5 that means:

$$a^2_1 = \sigma\left(\sum_i w^2_{1i}\, x_i + b^2_1\right) \tag{3.39}$$

However it is more convenient to stop considering every node individually and to view the involved quantities as vectors and matrices. So that (3.39) can be written as:

$$\mathbf{a}^l = \sigma\left(\hat{\mathbf{w}}^l \mathbf{a}^{l-1} + \mathbf{b}^l\right) \tag{3.40}$$



(a) rectified linear unit (ReLu)

(b) sigmoid

Figure 6: Two examples of activation functions σ. Especially the relu function has a destinct on and off state similar to a biological neurons.

5.font is wrong

Training During training the network output $\mathrm{NN}(\mathbf{x}) := \mathbf{y}'$ is calculated through repeated use of (3.40) and is then compared with the known correct output $\mathbf{y}$ by a cost function $C = C(\mathbf{y}, \mathbf{y}')$. The goal of the training is to minimize this function C. The cost function might simply be the mean squared difference between $\mathbf{y}$ and $\mathbf{y}'$:

$$C_{\mathrm{mse}}(\mathbf{y}, \mathbf{y}') = \sum_i \left(y_i - y_i'\right)^2 \tag{3.41}$$

but there are different cost functions for different kind of outputs. For example a network which predicts continuous values needs a different loss than one predicting categories. More on this in section 4.1. Now we can quantify how well the NN is performing but how should the weights and biases be changed to improve this performance? Here the Algorithm *Backpropagation* is used and allows an efficient calculation of $\nabla C_{\mathbf{b}^l}$ and $\nabla C_{\hat{\mathbf{w}}^l}$ **6.explain backprop**. These are used to gradually change the weights and biases to minimize the cost function. A comprehensive explanation of Backpropagation can be found here: [1].

Convolutional Neural Networks An area where NNs have been very successful is image recognition or more general computer vision but the described multilayer perceptron has a number of weaknesses for this kind of task. Let's say our input is a n by n gray scale image. This can be expressed as a $n \times n$ matrix, flattened and fed into the input layer (see figure 7). But now the number of weights to the next layer $\hat{\mathbf{w}}^2$ is $n \cdot n \cdot \left|\boldsymbol{l}^2\right|$ which soon becomes unfeasible. As described in the section on notation $\boldsymbol{l}^2$ is here the activation vector of the second layer and not $\boldsymbol{l}$ squared.

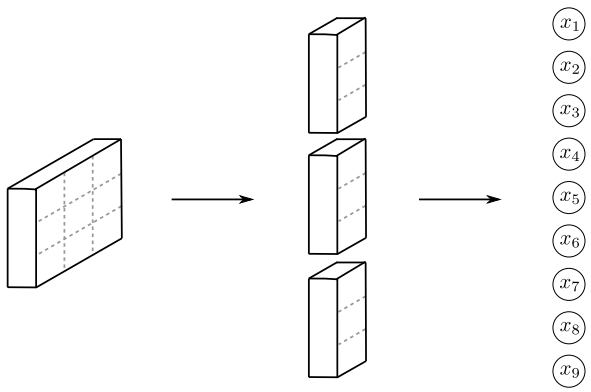


Figure 7: Flattening of a 3×3 matrix to fit the input of a multilayer perceptron.

Computational limits aside there is another problem. Imagine an image with the letter T in the top right corner. If this letter moves to a different position as in figure 8 the networks reaction will be completely different because the weights and biases involved are completely different. So the NN cannot learn the concept "letter T" independent of its position in the picture. Also the information about the distance between pixels is lost.

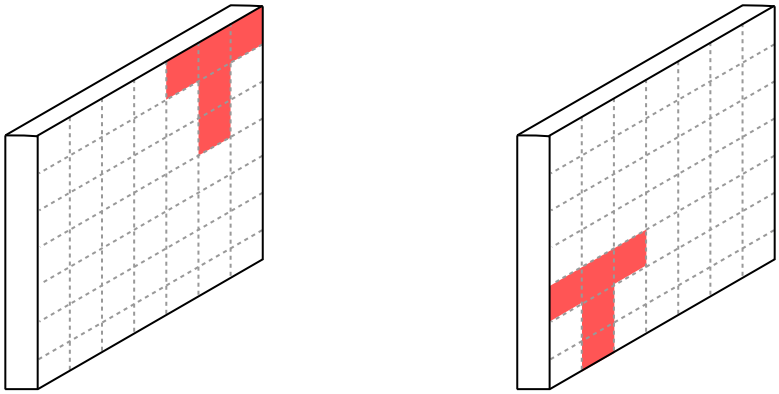


Figure 8: Two pictures of a T at different positions where the red color signifies a high value in the grayscale image. After the flatten operation seen in figure 7 very different nodes are active.

These problems led to the development of a new kind of layer called *Convolution*. A fixed size squared matrix called *kernel* is shifted over the matrix and at every position the the point wise product between kernel and matrix is calculated and summed as shown in figure 9:

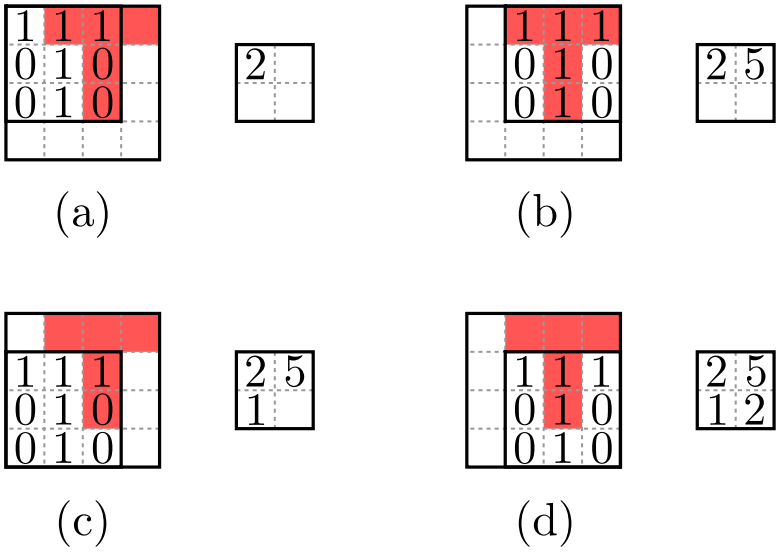


Figure 9: Example of a convolution. The 3×3 kernel is shifted over the image one step at the time. The red color in the image represents a pixel value of 1. For example in picture (a) the point wise product between kernel and image is zero everywhere except at two positions where a one in the kernel meets a one in the image. Because there are less valid positions for the kernel than pixels in the image the result is smaller in size.

The result of this operation called feature map of that kernel (see figure 10). Notice how the greatest value of the feature map is at the position of the letter T. So with only a small number of weights the convolution is able to detect the T independent of its position in the image. This is still slightly misleading because this "T kernel" was intentionally constructed to find the "T". In a real convolutional layer the kernel values are trained via Backpropagation similar to the weights of a Multilayer Perceptron as described in the paragraph Training.

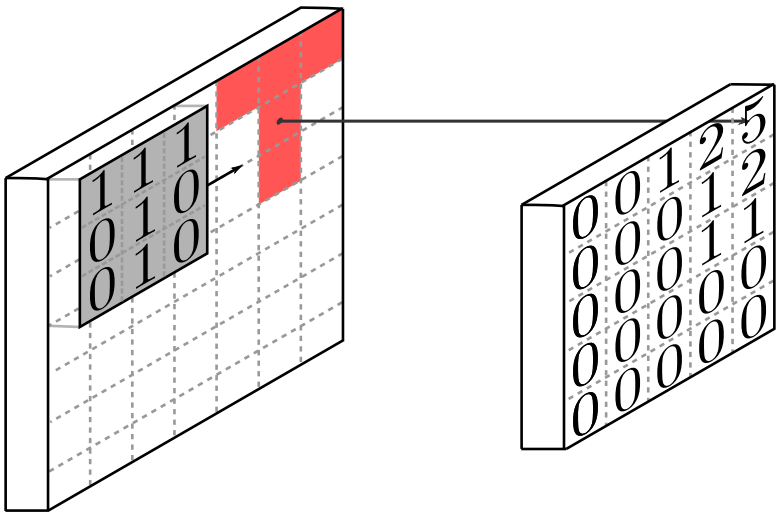


Figure 10: Example of a convolution where white pixel are 0 and red pixel are 1. The 3×3 Kernel is shifted over the image and when its directly over the The "T kernels" feature map is greatest at the position of the original letter.

One convolutional layer contains not only one but a number of different kernels k. The resulting k feature maps are stacked in the "z direction" so that the shape of the $n \times n$ matrix transforms to $(n-2) \times (n-2) \times k$. In a Convolutional Network (ConvNet) multiple of these layers are used so that it can find "patterns in patterns". For the letter detection example one could imagine the first layer to detect various edges and the next layer to detect letters in the position of these edges.

Pooling Layers For a big image and a large number of kernels the output shape of a convolutional layers is still $\mathcal{O}\big((n)^2 \cdot k\big)$, so quite large. Also notice how in figure 10 the "T kernel's" feature map is not only active at the exact position of the T but in the general region. The solution to this is to downsample the output with a *Pooling Layer*. Here a smaller kernel, usually 2×2 is shifted over the matrix two steps at a time and at every position an operation is performed to reduce the number of values to one. This could be taking the maximum or the average of that 2×2 region. This operation reduces the matrix in the x and y dimension by a factor of 2 as shown in figure 11:

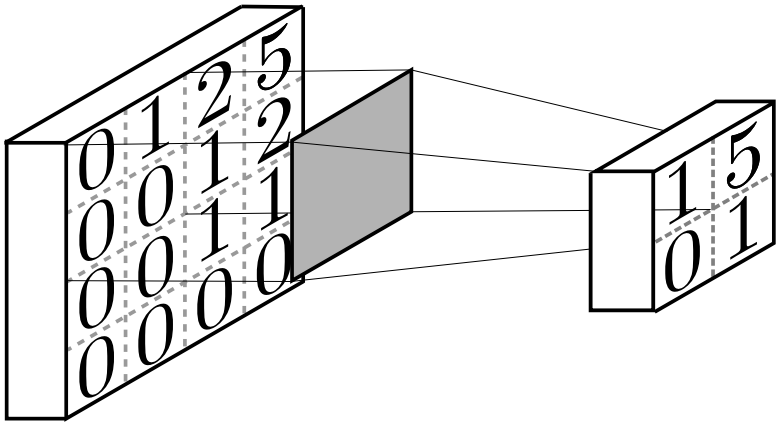


Figure 11: Example of a Max Pooling Layer. For every 2 by 2 field the maximum is calculated. After applying first the convolution and then the pooling layer the information "T in the top right corner" is still there and size of the resulting matrix is very manageable.

Example Network Architecture Now all the building blocks for a complete ConvNet are available. Repeatedly alternating convolution and pooling layers changes the input from wide in x and y dimension and narrow in z to a long z-strip. At the very end this strip is fed into one densely connected layer which is in turn connected to the output neurons. An example architecture of this kind is shown in

figure 12:

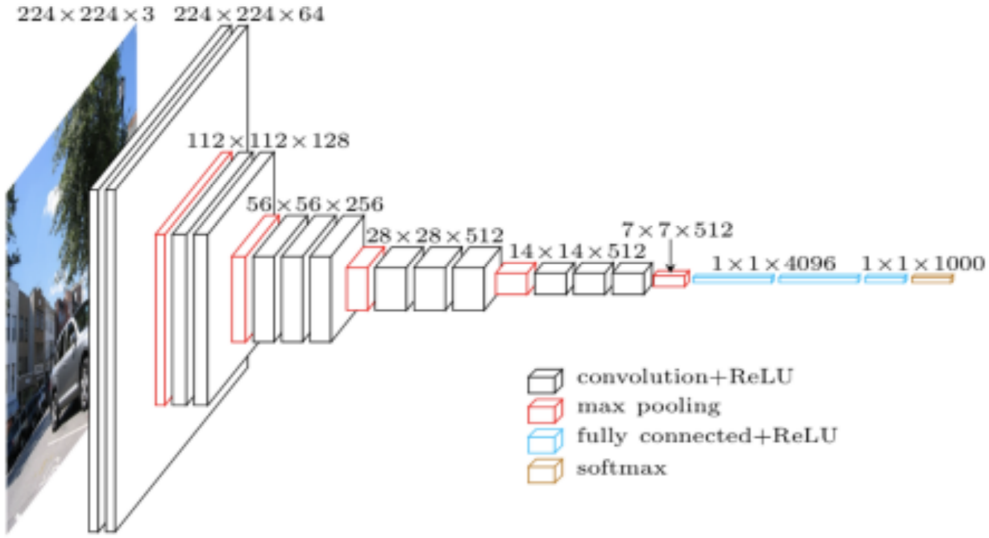


Figure 12: Example for a complete ConvNet. Note the input is in this case an RGB image so there are three layers in the z dimension corresponding to the different colors. In this case the first layer has 64 kernels of size $3 \times 3 \times 3$. The next convolution then has 128 kernels of size $3 \times 3 \times 64$. [citation needed]

1D ConvNets The input to the desired algorithm is a target spectrum to which the Network should output some parameters (more on this in the section 4.1). This input data is a function $I(\lambda)$ so only one dimensional but all the same ideas apply. Convolutional kernels are sized $1 \times 3 \times z$ and pooling kernels are $1 \times 2 \times z$. Both are only shifted in one direction as see in figure 13. These 1D convolutions might detect features like rising and falling edges and the later layers might combine these features into concepts like peaks and troughs but as always in machine learning what the network actually does to reach its objective is not controlled by the programmer.

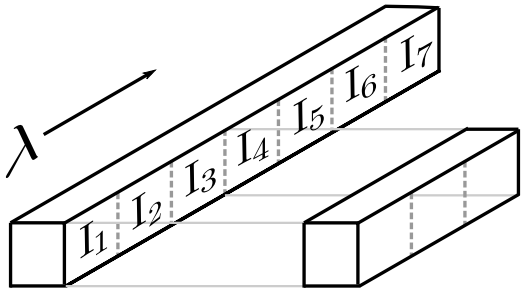
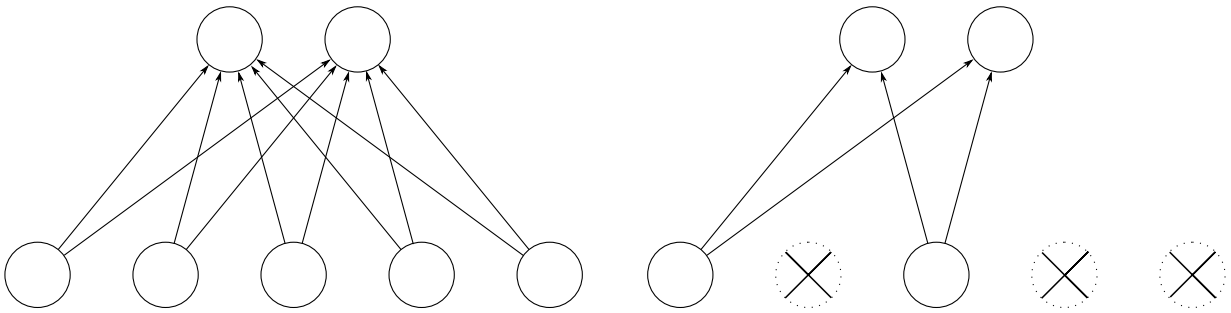


Figure 13: Example of a 1D convolution. A 1×3 kernel is shifted over a spectrum I discretized at 9 wavelengths

Dropout Layer In 2014 Srivastava et al.[2] presented a method to prevent overfitting and speed up the training process of large Neural Networks. During training they randomly drop a number of neurons in a layer along with all connections to and from these neurons. This prevents the neurons from co-adapting **7.explain co-adapting** and because there are less weights and biases to tune for each step the training becomes overall faster. The process of dropping some neurons is shown in figure 14:



(a) no dropout (b) with dropout

Figure 14: Example of a dropout applied to the bottom layer. Only two of the neurons remain active and only their weights and biases are modified during this training step. Figure found in [2] (modified)