Lecture 23: Review of Machine Learning + Imaging

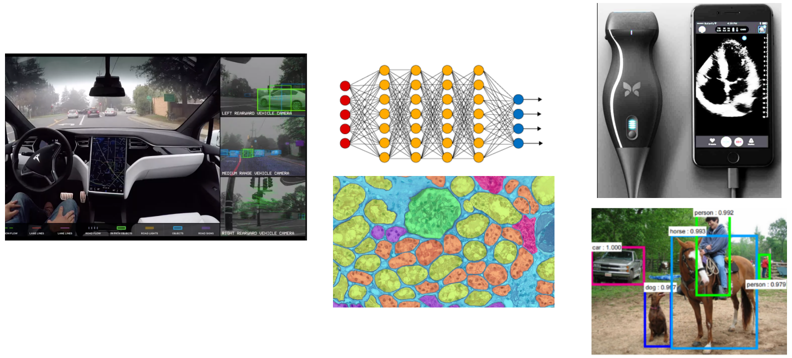
Machine Learning and Imaging

BME 590L
Roarke Horstmeyer

What was this class about?

Where your final project is aimed

Computer-
centered hardware + software



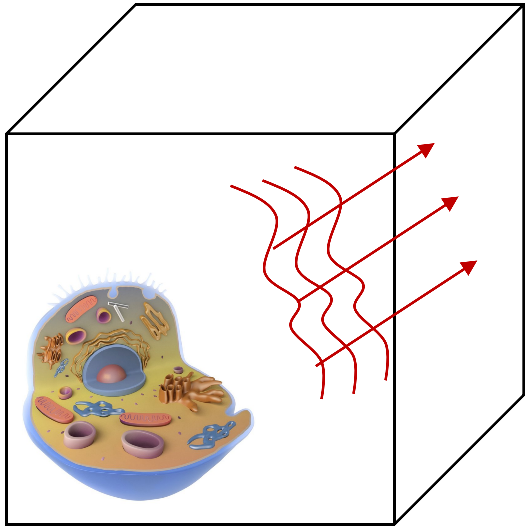
Human-centered hardware design

Computer-centered software design

deep imaging

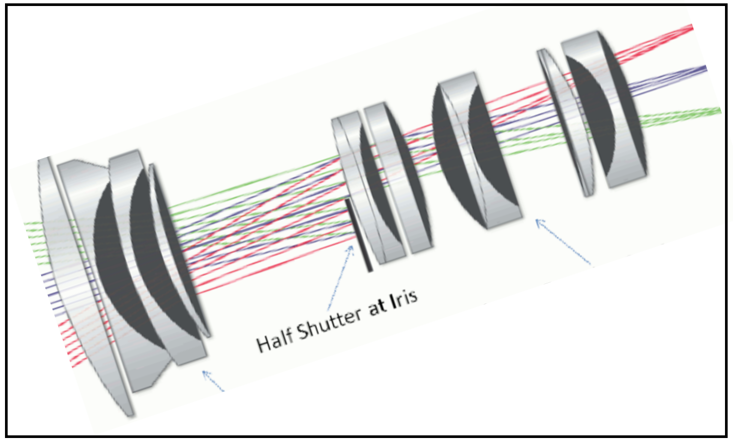
ML+Imaging pipeline introduction

Real World



Continuous
complex fields

Measurement device

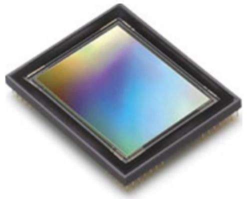


Black box transformations

- Convolution
- Fourier Transform

Digitization

γ -> e^-

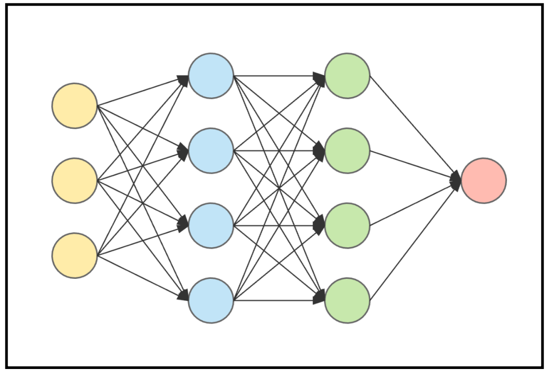


Sampling
Theorem

Discrete math &
Linear algebra

Summarize with simple models

Machine Learning



Optimization

Linear classification

Logistic classifier

Neural networks

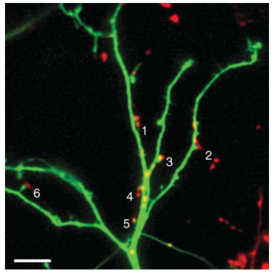
Convolutional NN's

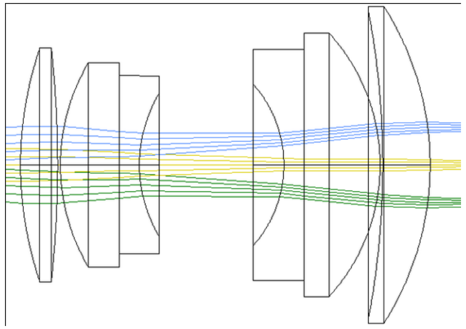
Use Tensorflow

Physical models for light propagation to sensor

deep imaging

- **Interpretation #1: Radiation (*Incoherent*)**
- Model: Rays



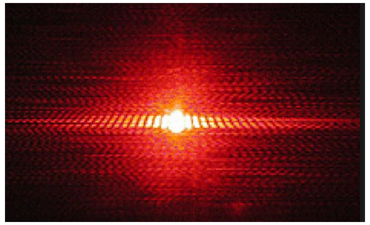


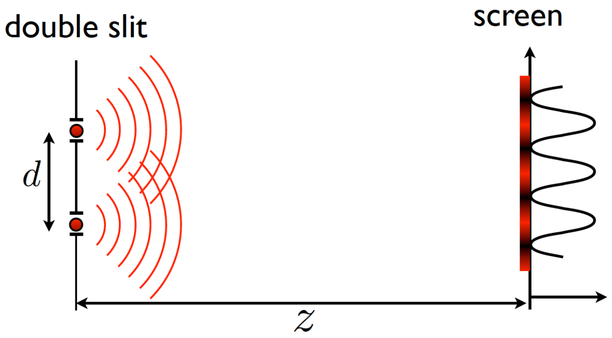
- Real, non-negative

$$\boxed{I_s = H\,B\,S_0}$$

- Sample absorption **S**
- Illumination brightness **B**
- Blur in **H**

- **Interpretation #2: Electromagnetic wave (*Coherent*)**
- Model: Waves





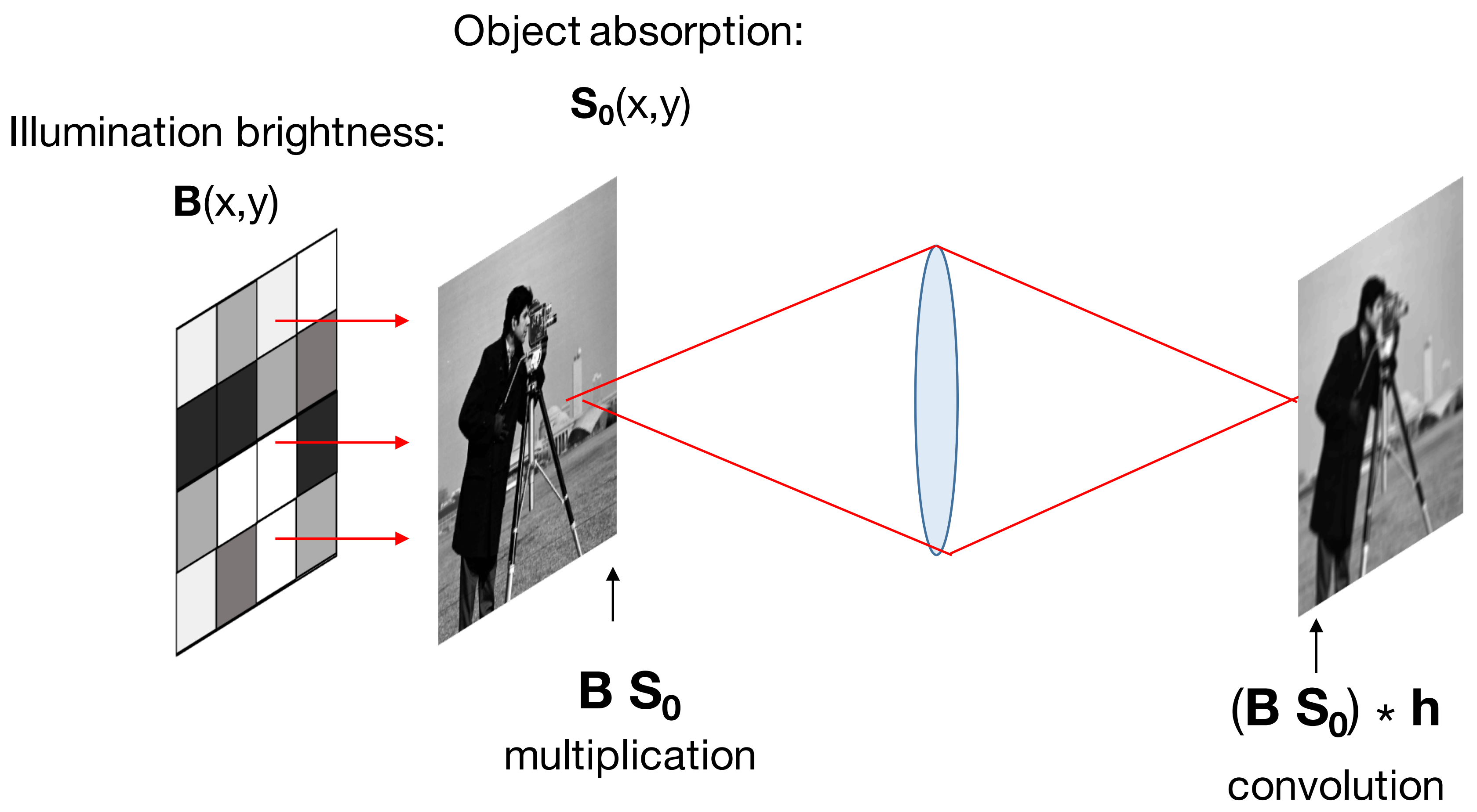
- Complex field

$$\boxed{I_C = |H\,C\,S_C|^2}$$

- Sample abs./phase **S**
- Illumination wave **B**
- Blur in **H**

Mathematical model of for incoherent image formation

- All quantities are real, and non-negative



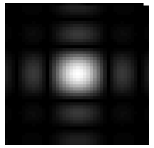
We can also add in some lens blur

Lenses blur and rescale images:

Input intensity

Convolution filter h

$*$



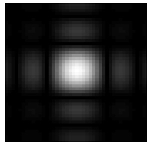
"Incoherent point-spread function"

$=$

Output intensity

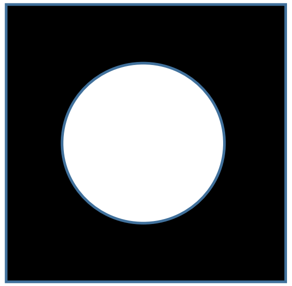
$h(x,y) = | F[A(f_x,f_y)] |^2$

h(x,y)



$= | F [$

A(f_x,f_y)



$] |^2$

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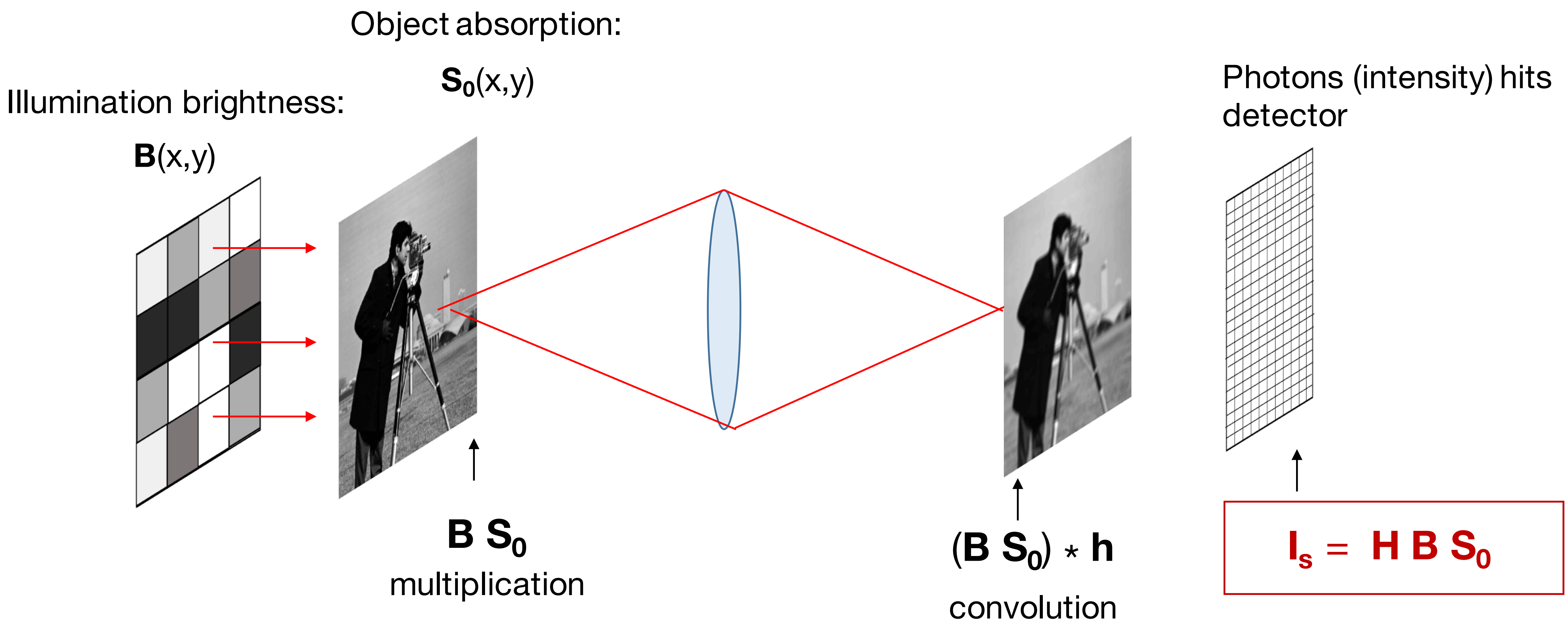
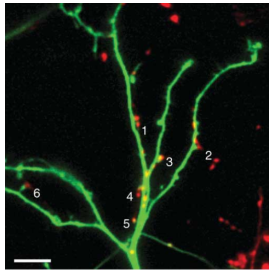
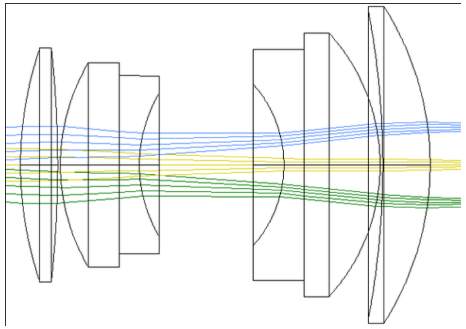


Physical models for light propagation to sensor

- **Interpretation #1: Radiation (*Incoherent*)**
- Model: Rays





- Real, non-negative

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- **Interpretation #2: Electromagnetic wave (*Coherent*)**
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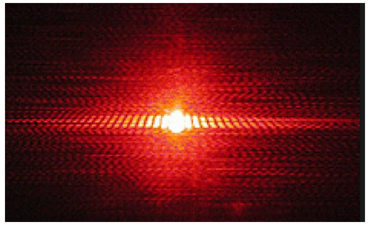

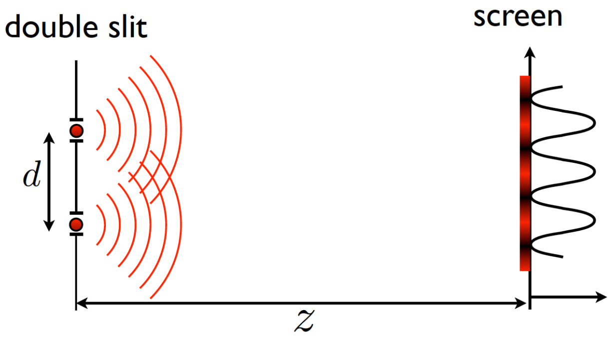

- Complex field

$$\boxed{I_C = |\,H\,C\,S_C|^2}$$

- Sample abs./phase **S**
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- Blur in **H**

Let's take a step back: how does light propagate?

Maxwell's equations without any charge

$$\nabla \times \vec{\mathcal{E}} = -\mu \frac{\partial \vec{\mathcal{H}}}{\partial t}$$

$$\nabla \times \vec{\mathcal{H}} = \epsilon \frac{\partial \vec{\mathcal{E}}}{\partial t}$$

$$\nabla \cdot \epsilon \vec{\mathcal{E}} = 0$$

$$\nabla \cdot \mu \vec{\mathcal{H}} = 0.$$

1. Take the curl of both sides of first equation
2. Substitute 2nd and 3rd equation
3. Arrive at the wave equation:

$$\nabla^2 \vec{\mathcal{E}} - \frac{n^2}{c^2} \frac{\partial^2 \vec{\mathcal{E}}}{\partial t^2} = 0 \qquad n = \left(\frac{\epsilon}{\epsilon_0}\right)^{1/2} \qquad c = \frac{1}{\sqrt{\mu_0 \epsilon_0}}.$$

Let's take a step back: how does light propagate?

Considering light that isn't pulsed over time, we can use the following solution:

$$u(P, t) = A(P)\cos[2\pi\nu t + \phi(P)]$$

$$u(P, t) = Re\{U(P)\exp(-j2\pi\nu t)\},$$

With this particular solution, we get the following important time-independent equation:

Helmholtz Equation

$$\boxed{(\nabla^2 + k^2)U = 0.} \qquad k = 2\pi n\frac{\nu}{c} = \frac{2\pi}{\lambda},$$

This is an important equation in physics. We won't go into the details, but it leads to the Huygen-Fresnel principle:

$$U(P_2) = \frac{1}{j\lambda}\iint_{\Sigma} U(P_1)\frac{\exp(jkr_{21})}{r_{21}}\cos\theta\, ds$$

From the Fresnel approximation to the Fraunhofer approximation

deep imaging

Fresnel Approximation:

$$E(x,y,z) = \frac{e^{ikz}}{i\lambda z} \iint_{-\infty}^{+\infty} E(x',y',0) e^{\frac{ik}{2z}\left[(x-x')^2+(y-y')^2\right]} dx' dy'$$

Lets assume that the second plane is "pretty far away" from the first plane. Then,

$$\boxed{z > \frac{2D^2}{\lambda}}$$

1. Expand the squaring

$$E(x,y,z) = \frac{e^{ikz}}{i\lambda z} \iint E(x',y',0) e^{\frac{ik}{2z}(x^2+y^2)} e^{\frac{ik}{2z}(x'^2+y'^2)} e^{\frac{ik}{2z}(xx'+yy')} dx' dy'$$

2. Front term comes out, assume second term goes away, then,

$$\boxed{E(x,y,z) = C \iint E(x',y',0) e^{\frac{ik}{2z}(xx'+yy')} dx' dy'}$$

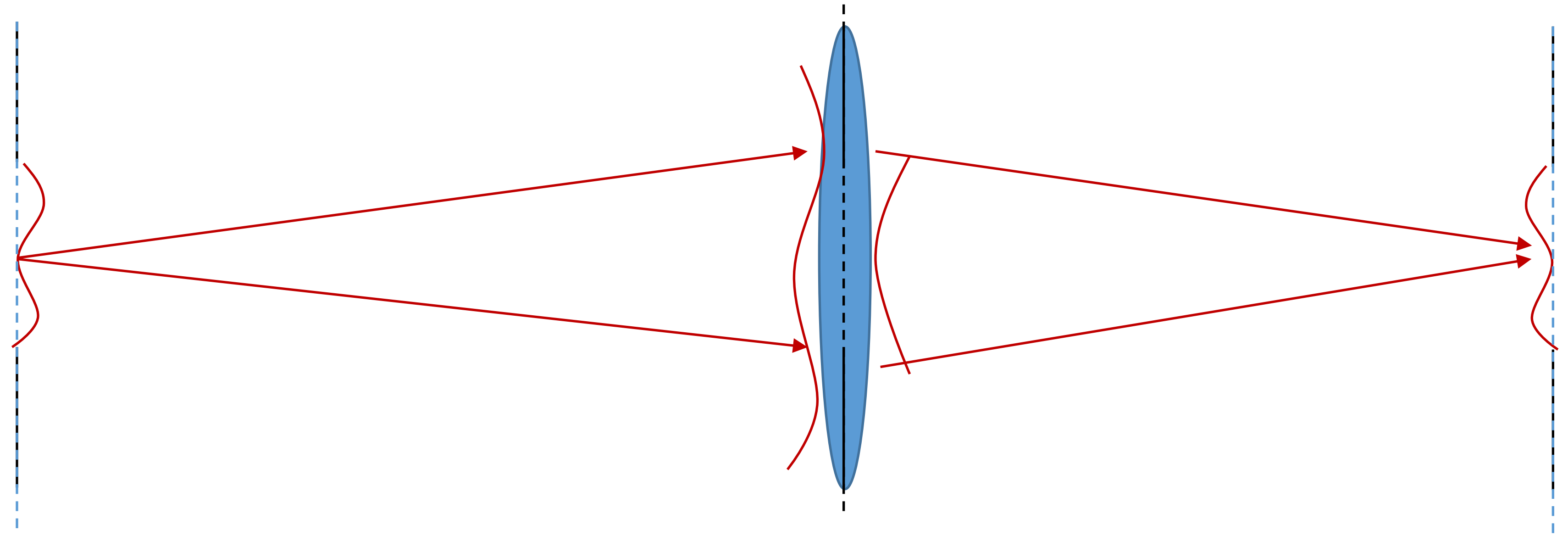
$$C = \frac{e^{ikz}}{i\lambda z} e^{\frac{ik}{2z}(x^2+y^2)}$$

Fraunhofer diffraction is a Fourier transform!!!!!!!

Model of a microscope (or camera) using Fourier transforms:

from lens to sensor, light undergoes an

inverse Fourier transform!



$$E_s(x_s, y_s, 0)$$

$$E'_a(x_d, y_d) = E_a(x_d, y_d)A(x_d, y_d)$$

2D Fourier Transform

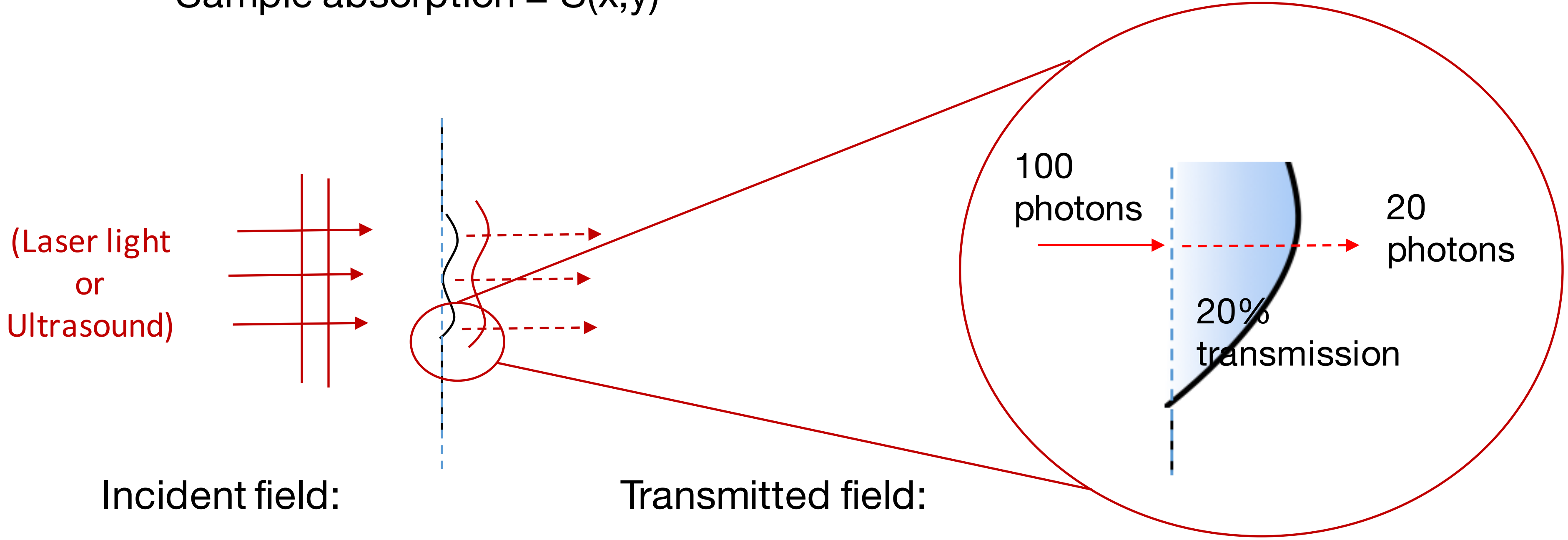
2D inverse Fourier Transform

Mathematical model of for coherent image formation

- Pretty much the same thing, but now we have an amplitude and a complex phase

Sample absorption = S(x,y)

Point #1: Amplitudes behave just like before



$$A_t(x,y) = A_i(x,y)\, S(x,y)$$

Incident field:

$$C(x,y) = A_i(x,y)$$

Transmitted field:

$$U(x,y) = A_t(x,y) = A_i(x,y)\, S(x,y)$$

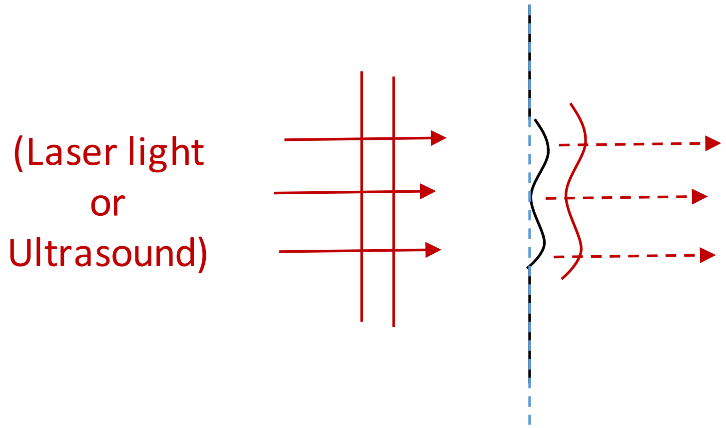
Mathematical model of for coherent image formation

- Pretty much the same thing, but now we have an amplitude and a complex phase

Sample absorption = S(x,y)

Sample phase delay = $\exp[ik\varphi(x,y)]$

New: complex phase delay
- Needed to represent wave
- Represents wave delay across space



Incident field:

$C(x,y) = A_i(x,y)\ \exp[ik\varphi_i(x,y)]$

Transmitted field:

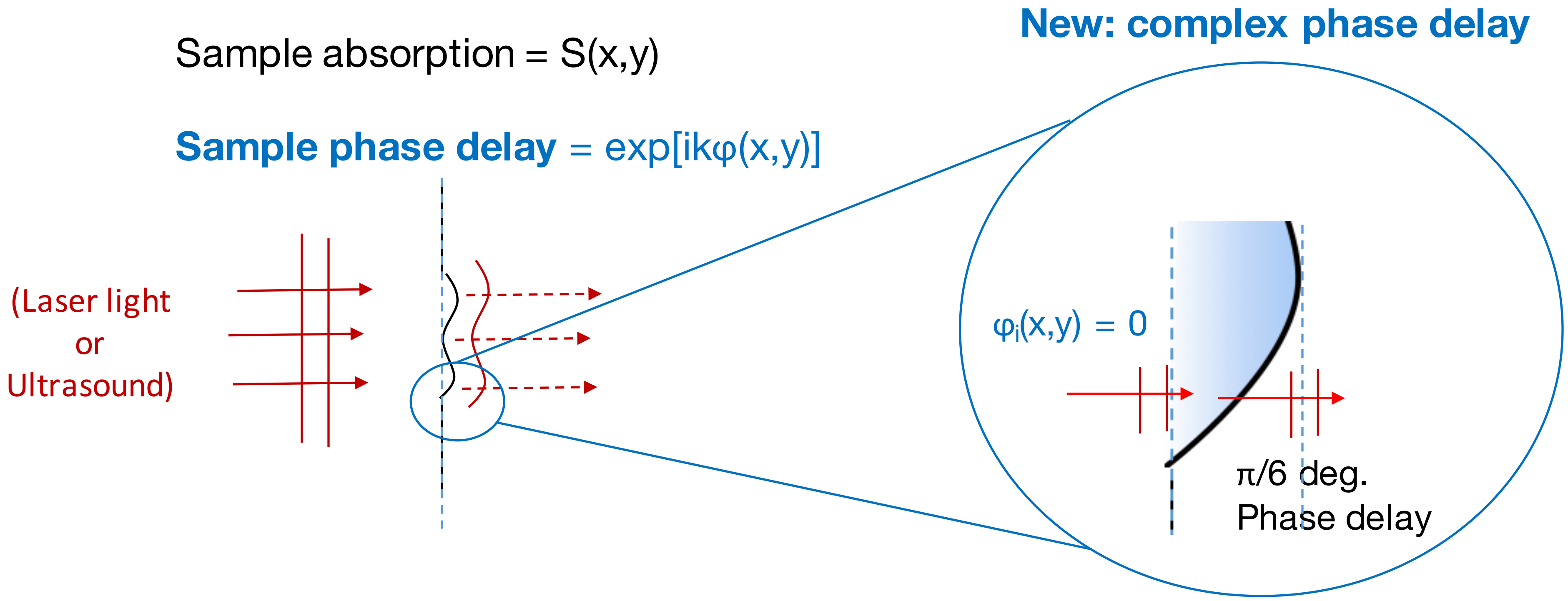
$U(x,y) = A_i(x,y)\ S(x,y)\ \exp[ik\varphi_t(x,y)]$

Mathematical model of for coherent image formation

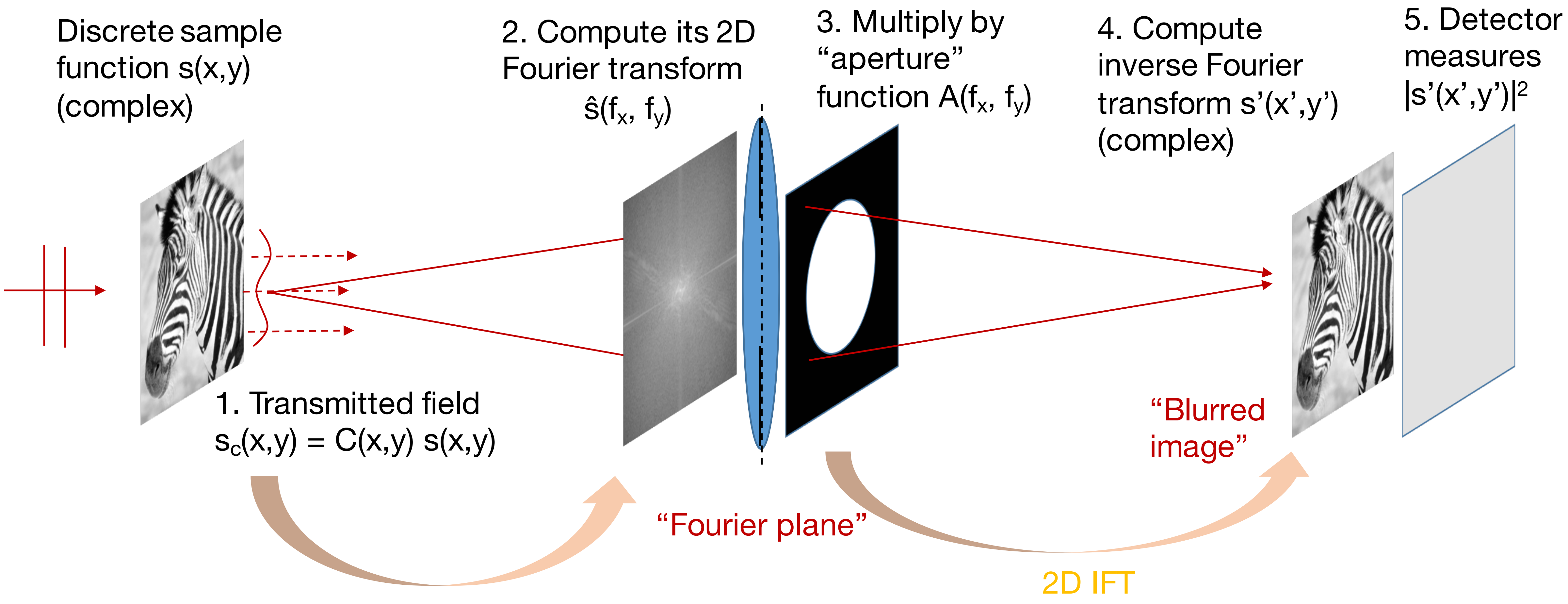
- Pretty much the same thing, but now we have an amplitude and a complex phase

Sample absorption = S(x,y)

Sample phase delay = $\exp[ik\varphi(x,y)]$

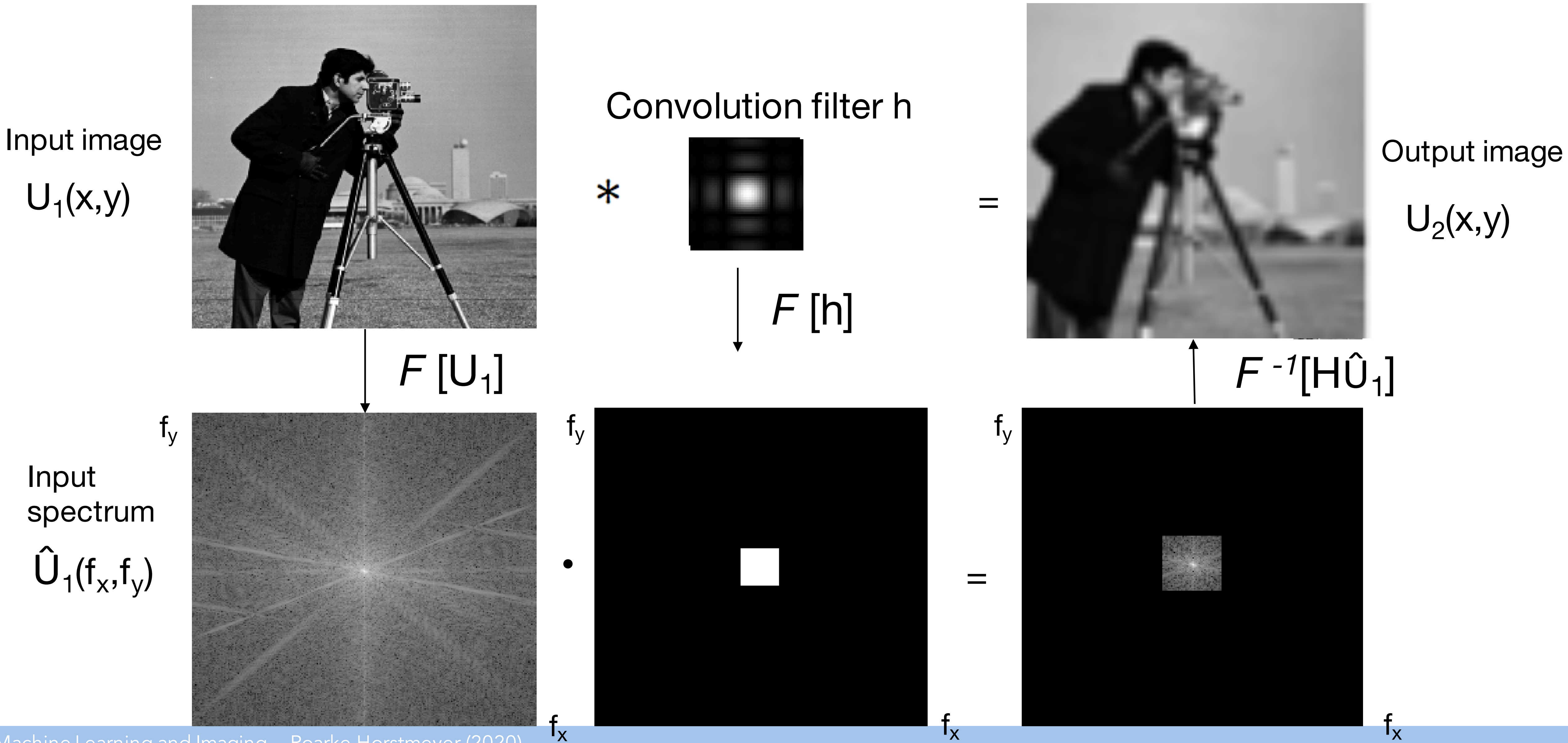


Model of image formation for wave optics (coherent light):



$$\boxed{\text{Model \#1: } I_c(x,y) = |F^{-1}AFCs|^2}$$

Coherent image blur – two implementations



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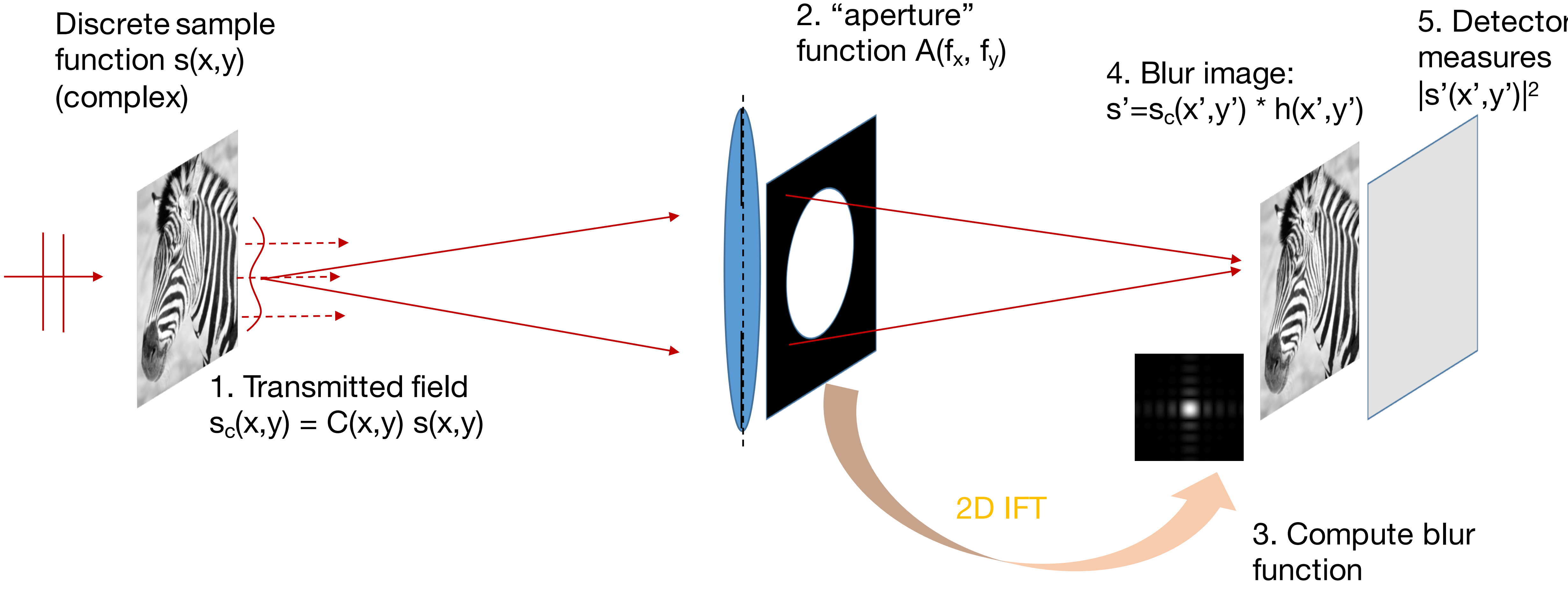
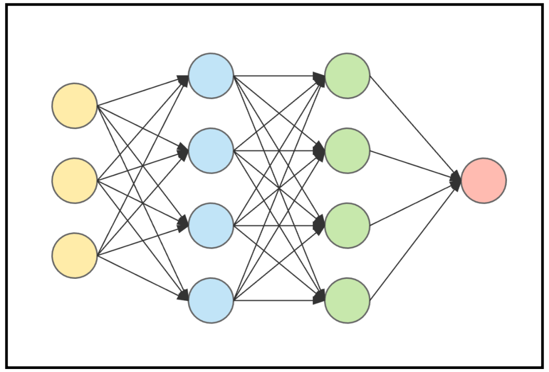
Model of image formation for wave optics (coherent light):



$$\boxed{\text{Model \#2: } I_c(x,y) = |h * Cs|^2}$$

Machine Learning

deep imaging



Optimization

Linear classification

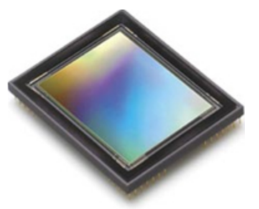
Logistic classifier

Neural networks

Convolutional NN's

Digitization

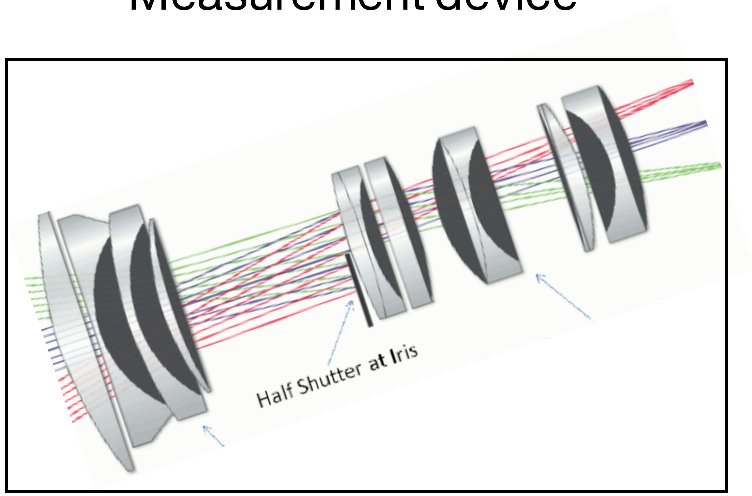
$\gamma \text{ -> } e^-$



Sampling Theorem

Discrete math & Linear algebra

Measurement device



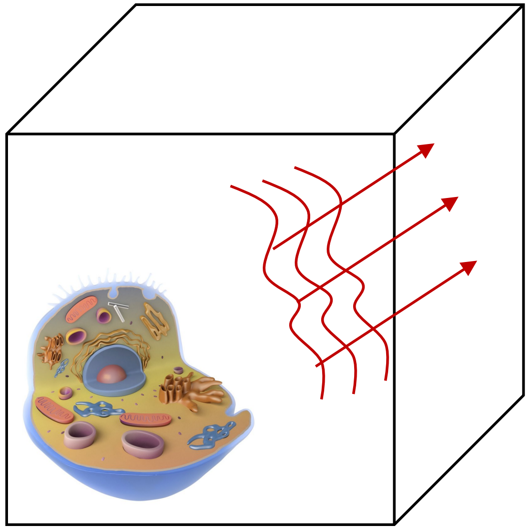
Black box transformations

- Convolution
- Fourier Transform

$$\boxed{I_{Inc} = H\ B\ S_0}$$

$$\boxed{I_{Coh} = |H\ C\ S_C|^2}$$

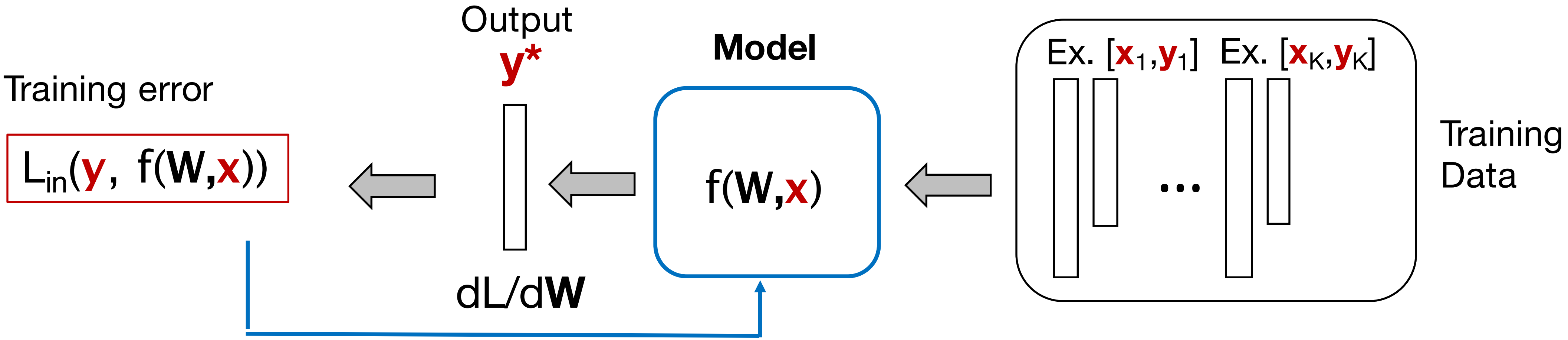
Real World



Continuous complex fields

Summary of machine learning pipeline:

1. Network Training



What we need for network training:

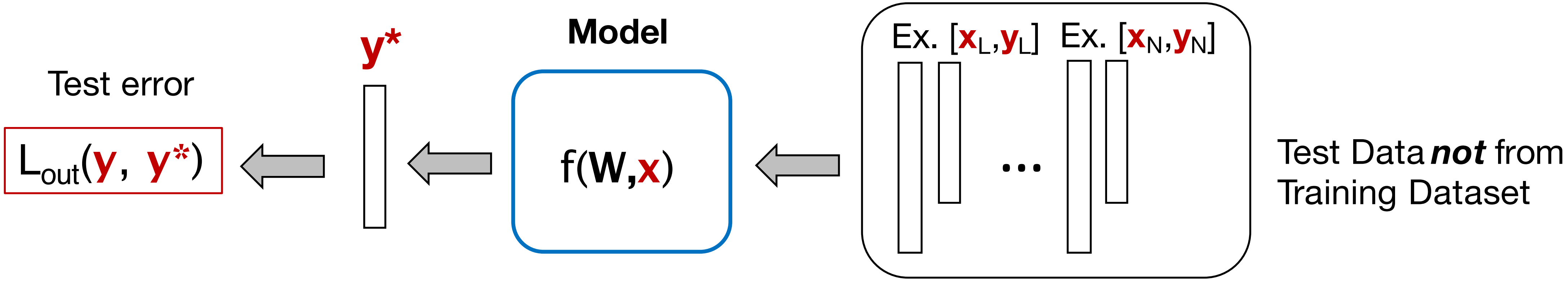
1. Labeled examples

2. A model and loss function

3. A way to minimize the loss function L

Summary of machine learning pipeline:

2. Network Testing



What we need for network testing:

4. *Unique* labeled test data
5. Evaluation of model error

Let's start with a simpler approach: linear regression

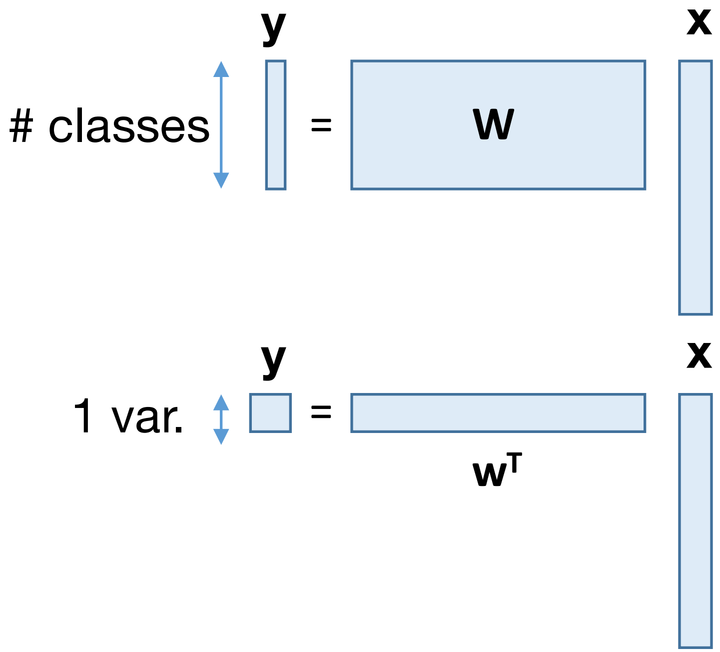
$$L = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, \mathbf{W}), y_i)$$

General linear model:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i(\mathbf{W}\mathbf{x}_i, y_i)$$

Assume 1 class =
1 linear fit

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i(w^T x_i - y_i)$$



Use MSE error
model

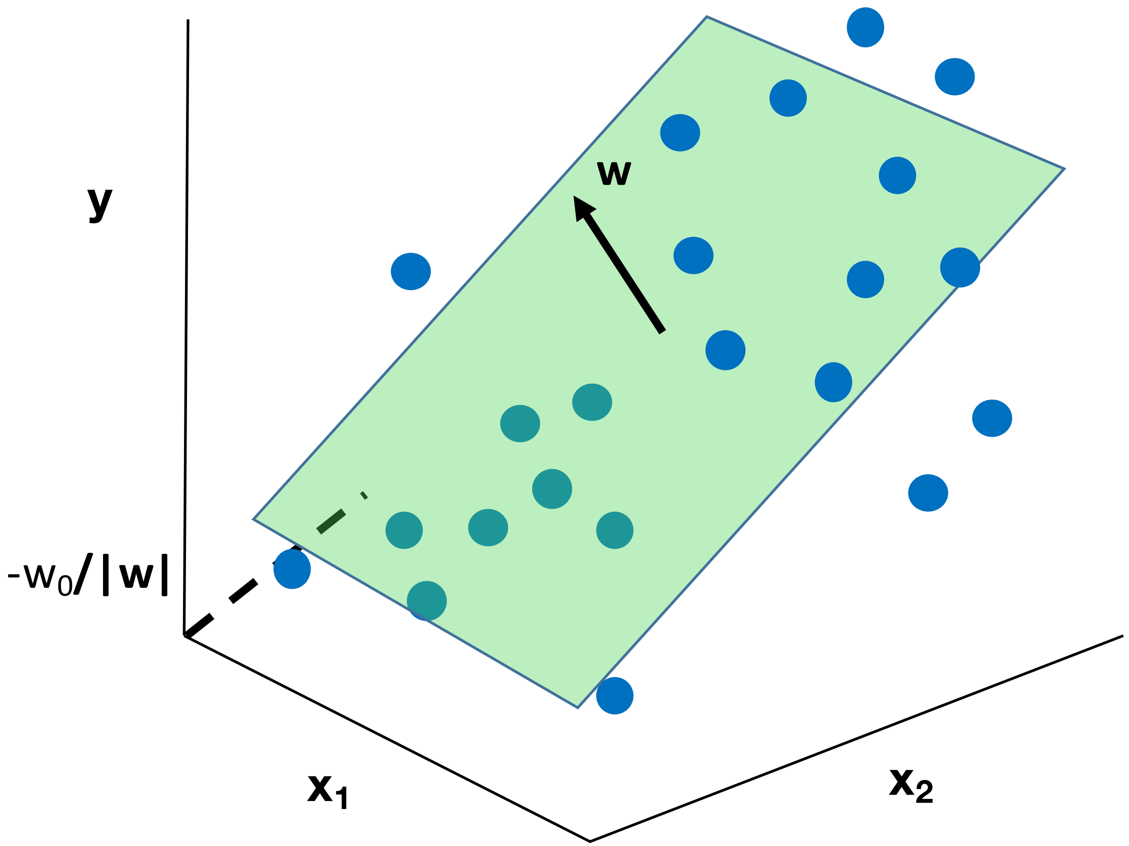
$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

Where labels
determined by
thresholding

$$f(\mathbf{x}_i) = y_i^* = \mathrm{sgn}(\mathbf{w}^T \mathbf{x}_i)$$

$$\mathrm{sgn}(x) := \begin{cases} -1 & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ 1 & \text{if } x > 0. \end{cases}$$

Why does linear regression with sgn() achieve classification?



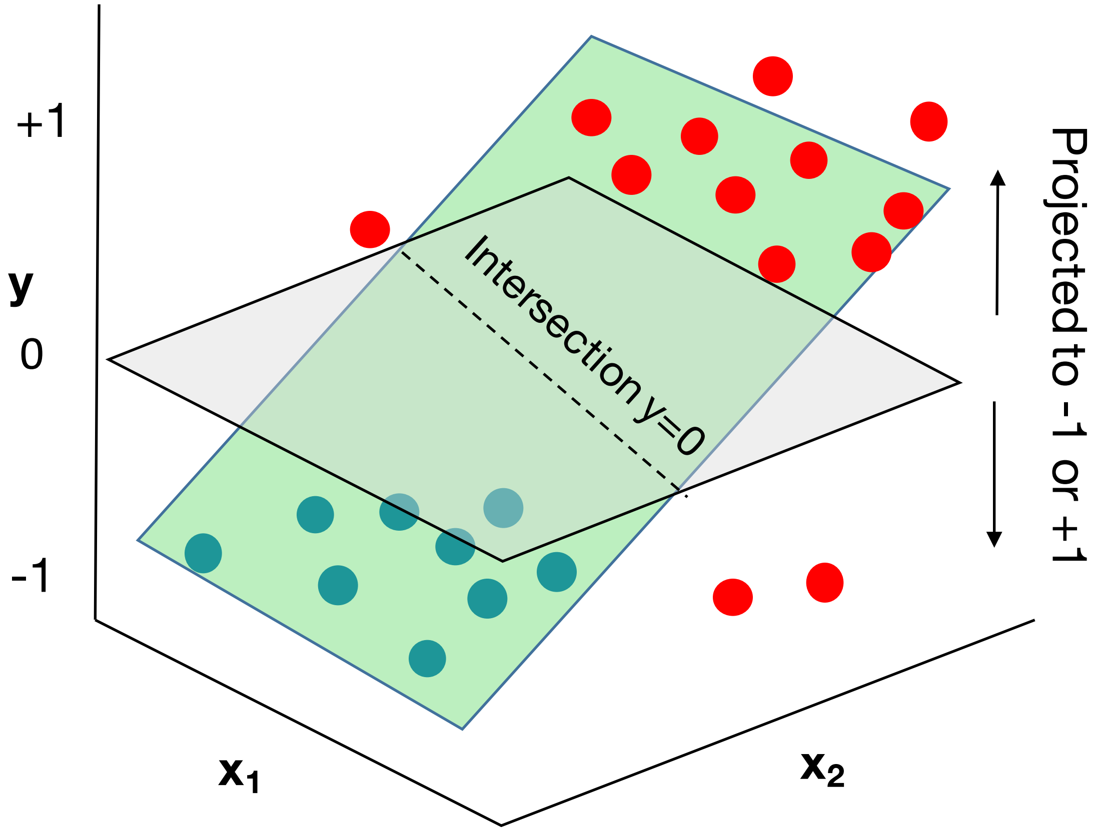
Without sgn(): regression for best fit

$$f(\mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i$$

$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

- If y_i can be anything, minimizing L makes **w** the plane of best fit

Why does linear regression with sgn() achieve classification?



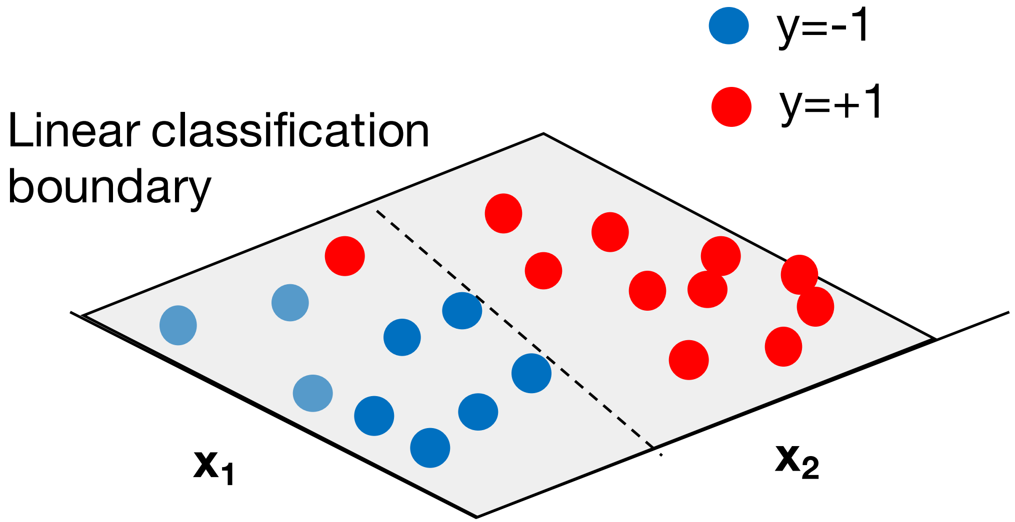
With sgn() operation:

$$f(\mathbf{x}_i) = y_i^* = \mathrm{sgn}(\mathbf{w}^T\mathbf{x}_i)$$

$$L = \frac{1}{N}\sum_{i=1}^{N}(w^T x_i - y_i)^2$$

- Anything point to one side of y=0 intersection is class +1, anything on the other side of intersection is class -1

Why does linear regression with sgn() achieve classification?



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$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

Sign operation takes linear regression and makes it a classification operation!

In the rest of this class: solve via gradient descent

With a matrix, compute this for each entry:

$$\boxed{\frac{dL(W_i)}{dW_i} = \lim_{h \to 0} \frac{L(W_i + h) - L(W_i)}{h}}$$

<u>Example:</u>

$W = [1,2;3,4]$
$L(W, x, y) = 12.79$

$W_1+h = [1.001,2;3,4]$
$L(W_1+h, x, y) = 12.8$

$dL(W_1)/dW_1 = 12.8\text{-}12.79/.001$

$\boxed{dL(W_1)/dW_1 = 10}$

- Repeat for all entries of **W**, dL/d**W** will have NxM entries for NxM matrix

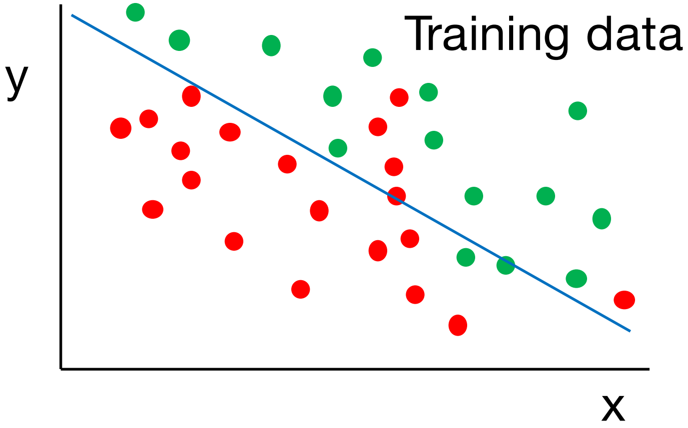
Steepest descent and the best step size ε

1. Evaluate function $f(\mathbf{x}^{(0)})$ at an initial guess point, $\mathbf{x}^{(0)}$
2. Compute gradient $\mathbf{g}^{(0)} = \nabla_{\mathbf{x}} f(\mathbf{x}^{(0)})$
3. Next point $\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \varepsilon^{(0)}\mathbf{g}^{(0)}$
4. Repeat – $\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} - \varepsilon^{(n)}\mathbf{g}^{(n)}$, until $|\mathbf{x}^{(n+1)}-\mathbf{x}^{(n)}| < \text{threshold } t$

$$L = \frac{1}{N}\sum_{i=1}^{N}(w^T x_i - y_i)^2$$

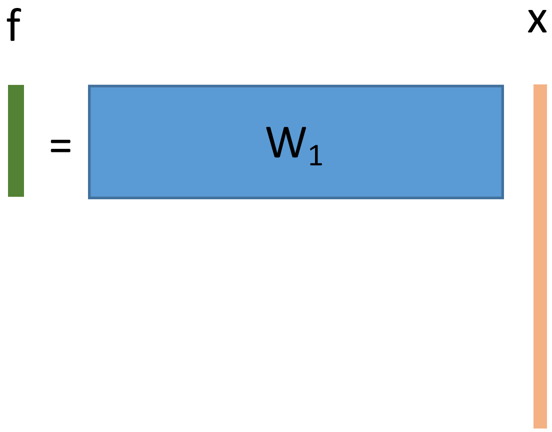
$$\nabla L(w) = \frac{2}{N} X^T (Xw - y) = 0$$

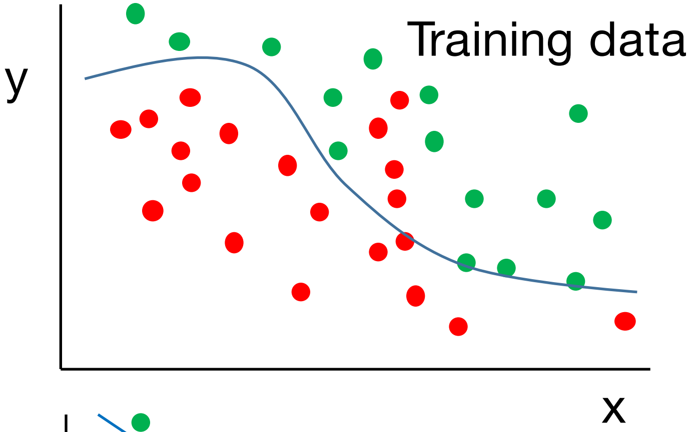
```
while previous_step_size > precision and iters < max_iters:
    prev_x = cur_x
    cur_x -= gamma * df(prev_x)
    previous_step_size = abs(cur_x - prev_x)
    iters+=1
```



$$f = W_1 x$$

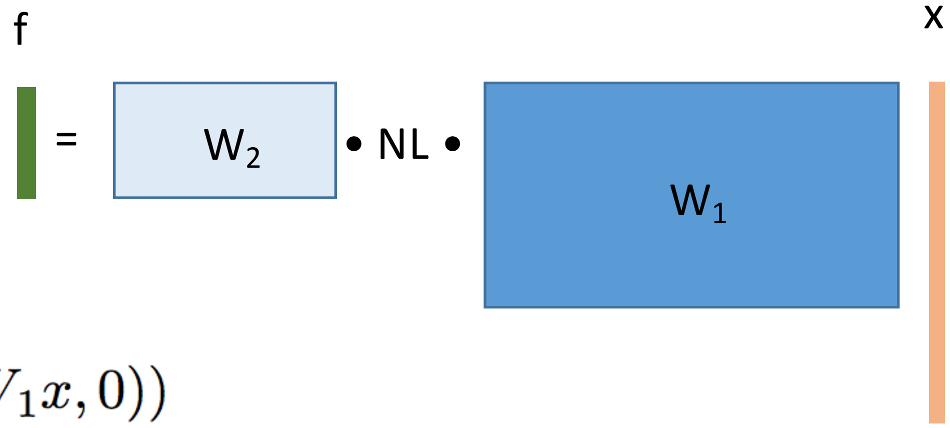
Learned *f:* not flexible

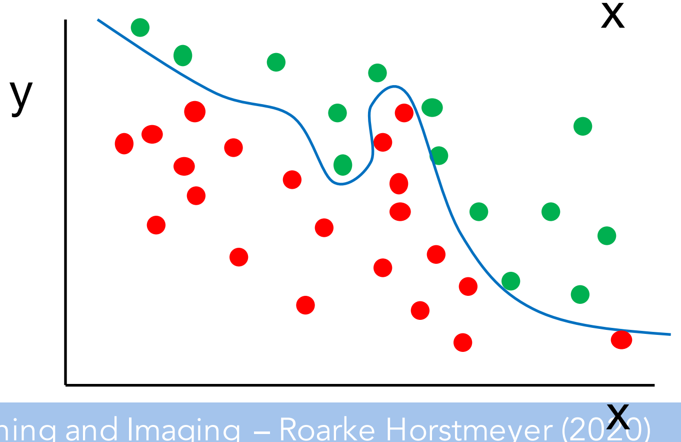




$$f = W_2 \max(W_1 x, 0)$$

Learned *f:* a bit flexible





$$f = W_3 \max(0, W_2 \max(W_1 x, 0))$$

Learned *f:* more flexible

Does it generalize???

We can keep adding these “layers”…

Before CNN's – understand two competing goals in machine learning

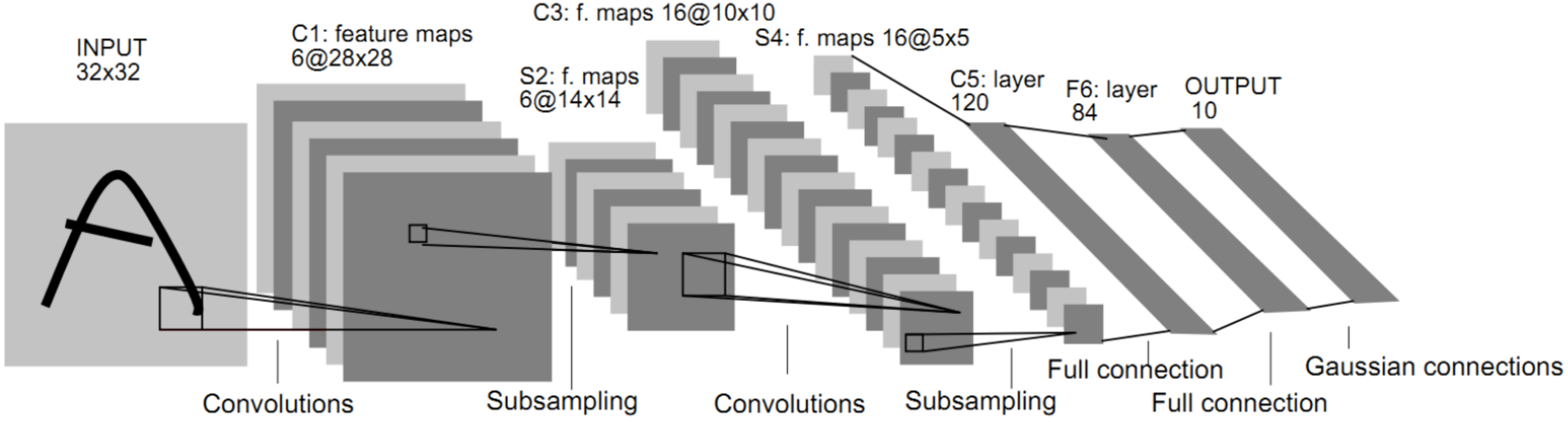
deep imaging

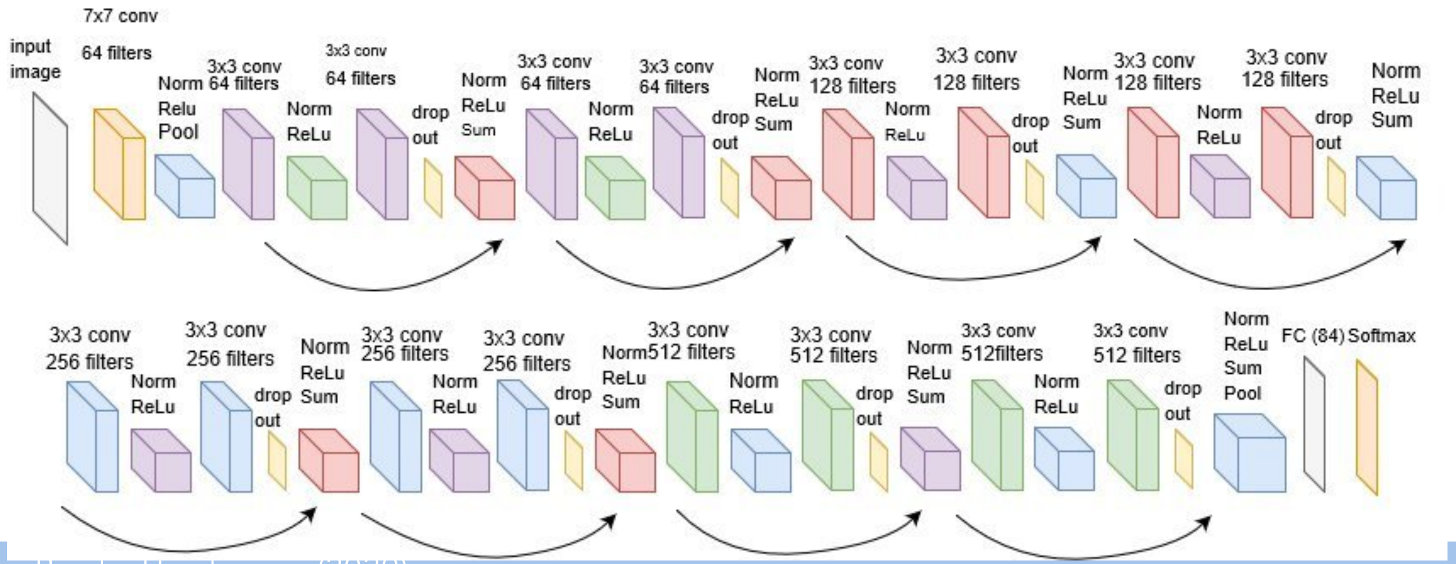
1. Can we make sure the in-sample error $L_{in}(y, f(x,W))$ is small enough?
   - Appropriate cost function
   - "complex enough" model

2. Can we make sure that $L_{out}(y, f(x,W))$ is close enough to $L_{in}(y, f(x,W))$?
   - Probabilistic analysis says yes!
   - $|L_{in} - L_{out}|$ bounded from above
   - Bound grows with model capacity (bad)
   - Bound shrinks with # of training examples (good)

Gets us to Convolutional Neural Networks

deep imaging





Important components of a CNN

deep imaging

CNN Architecture

- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers

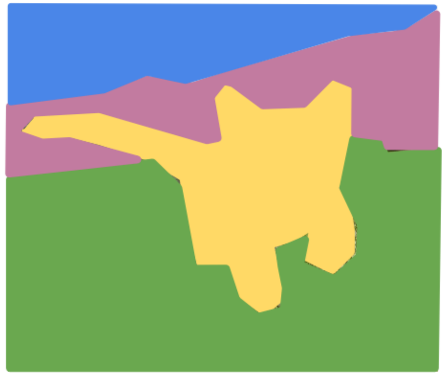
Loss function & optimization

- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

Other specifics: Pre-processing, initialization, dropout, batch normalization, augmentation

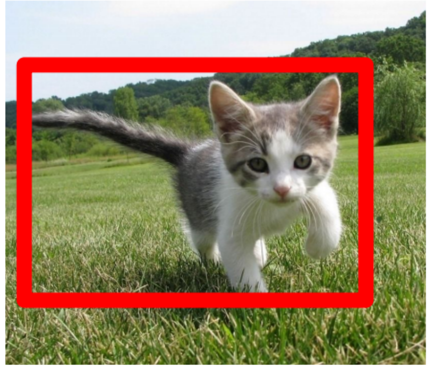
Other Computer Vision Tasks

Semantic Segmentation



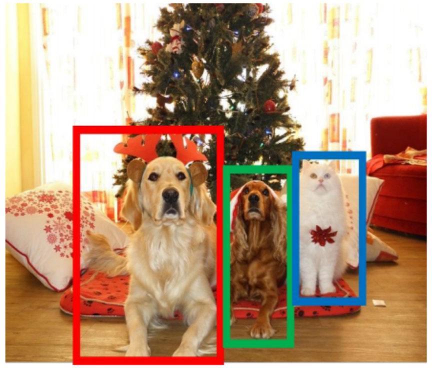
GRASS, CAT, TREE, SKY

Classification + Localization



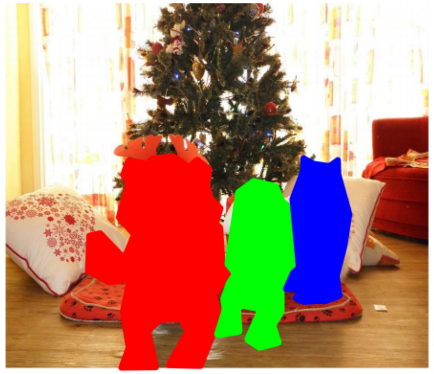
CAT

Object Detection



DOG, DOG, CAT

Instance Segmentation



DOG, DOG, CAT

Super-resolution

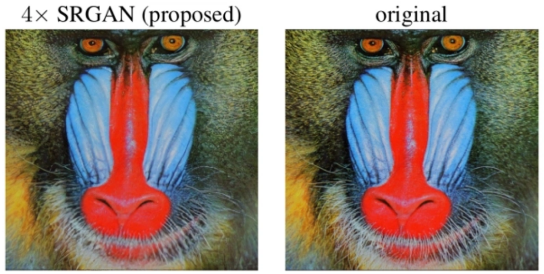


Figure 1: Super-resolved image (left) is almost indistinguishable from original (right). [4× upscaling]

No objects, just pixels

Single Object

Multiple Object

Post-processing of your results: a few options at different stages

Options to examine your test data after processing:

- ROC curve, Precision-Recall
- Confusion matrix
- Sliding window visualization
- Layer visualizations
- Saliency maps etc.
- tSNE visualization

Instead, *compress x-y dimensions of* input image

- Compress spatial features into learned filters
- Then, decompress learned filters back into same spatial dimensions
- **Can be an autoencoder**
- Analogous to image compression
- A very powerful idea…

U-Net: Convolutional Networks for Biomedical Image Segmentation

Olaf Ronneberger, Philipp Fischer, and Thomas Brox

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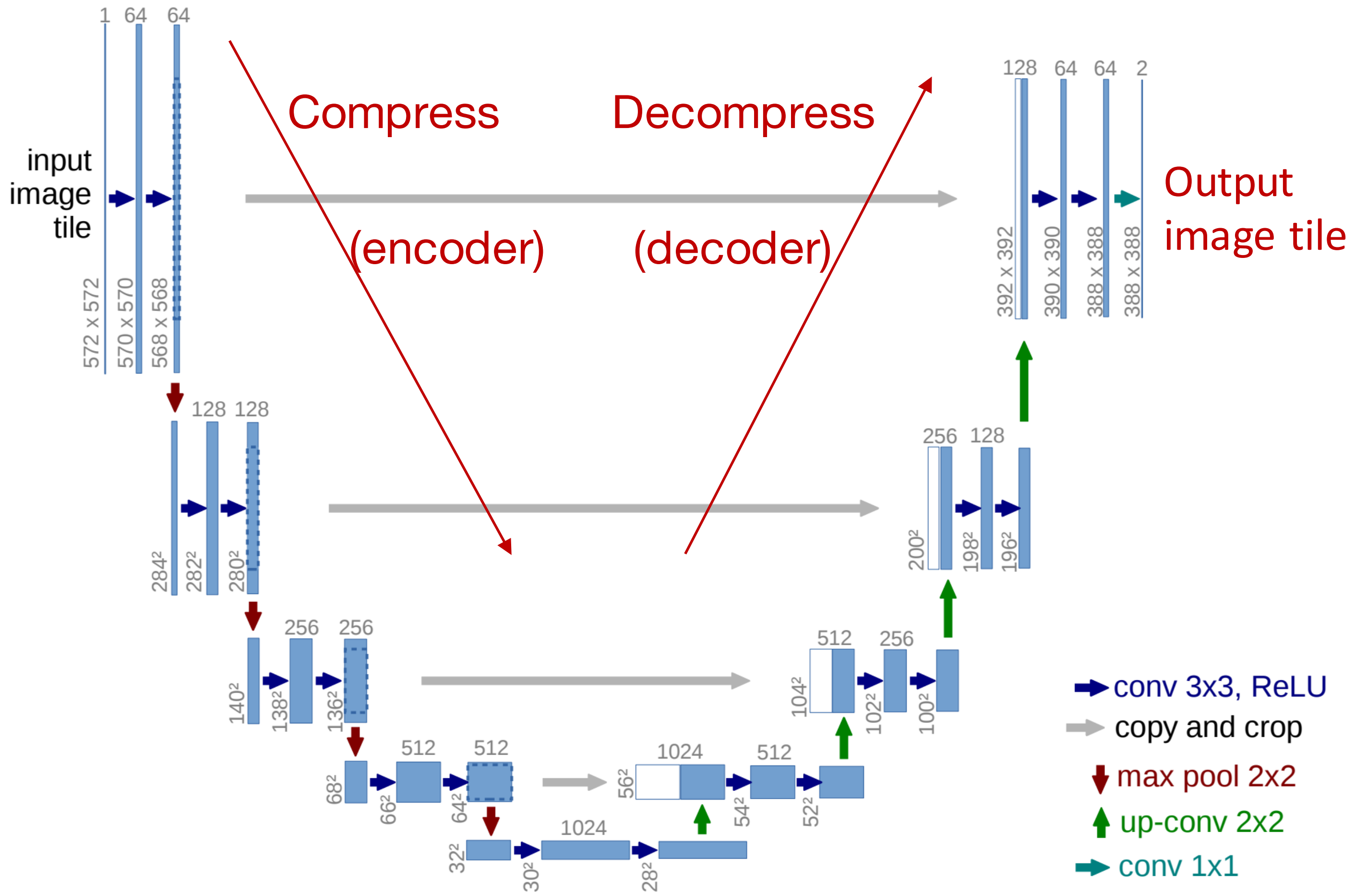
ronneber@informatik.uni-freiburg.de,
WWW home page: http://lmb.informatik.uni-freiburg.de/

U-Net Architecture



Bringing together physical and digital image representations

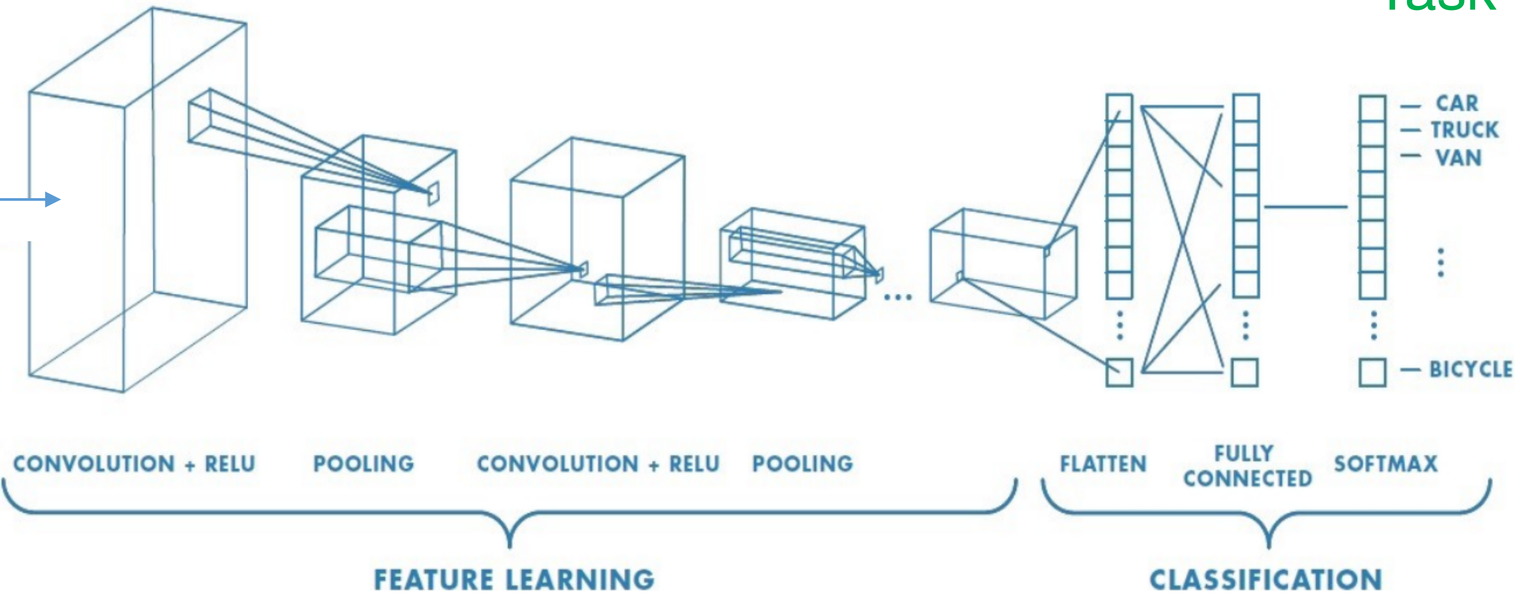
deep imaging

Physical Layers

Digital Layers

Task

Physical Function $\mathbf{I_0}$ → f[ ] → Digitized $\mathbf{I_s}$ →



$$\mathbf{I_s} = f[\mathbf{I_0}]$$

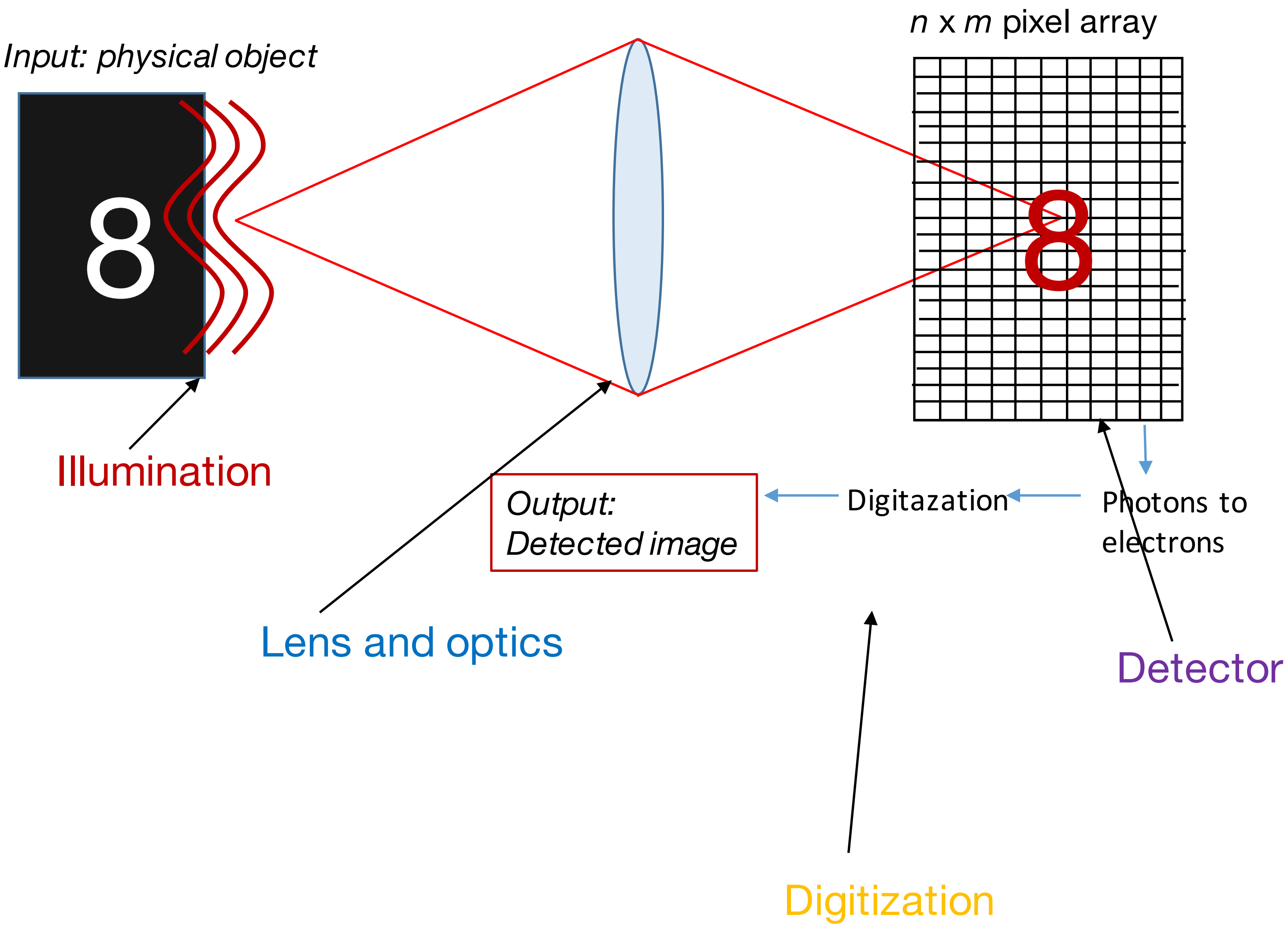
Digital layers

Physical layers

$$\text{Task} = \mathbf{W_n} \ldots \text{ReLU}[\mathbf{W_1}\ \text{ReLU}[\mathbf{W_0}\ f[\mathbf{I_0}]] \ldots]$$

What physical parameters effect image formation?

- Illumination
  - Spatial pattern
  - Angle of incidence
  - Color, polarization
- Lens and optics
  - Position/orientation
  - Shape
  - Focus
  - Transparency
- Detector
  - Pixel size
  - Pixel shape & fill factor
  - Color filters
  - Other filters
- Digitization
  - E to P curves
  - Digitization schemes/thresholds
  - Data transmission, multiplexing
- Physical object



Example code to achieve this is in Homework #5 and linked on course website:

deep imaging

jupyter physical_layers_example (unsaved changes)

File Edit View Insert Cell Kernel Help — Not Trusted — Python 3

In [2]:
```
import tensorflow as tf
import numpy as np
import matplotlib.pyplot as plt
tf.__version__
```
Out[2]: '2.0.0'

In [0]:
```
mnist = tf.keras.datasets.mnist
(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_test, x_train = x_test/255.0, x_train/255.0 # normalization
```

In [0]:
```
# add channel dimension, Tensorflow requests NHWC (or BHWC) format. Number/Batch_size, height, width, channels
# for 1D vectors, it should be Number/Batch_size, length
x_train = x_train[...,None]
x_test = x_test[..., None]
```

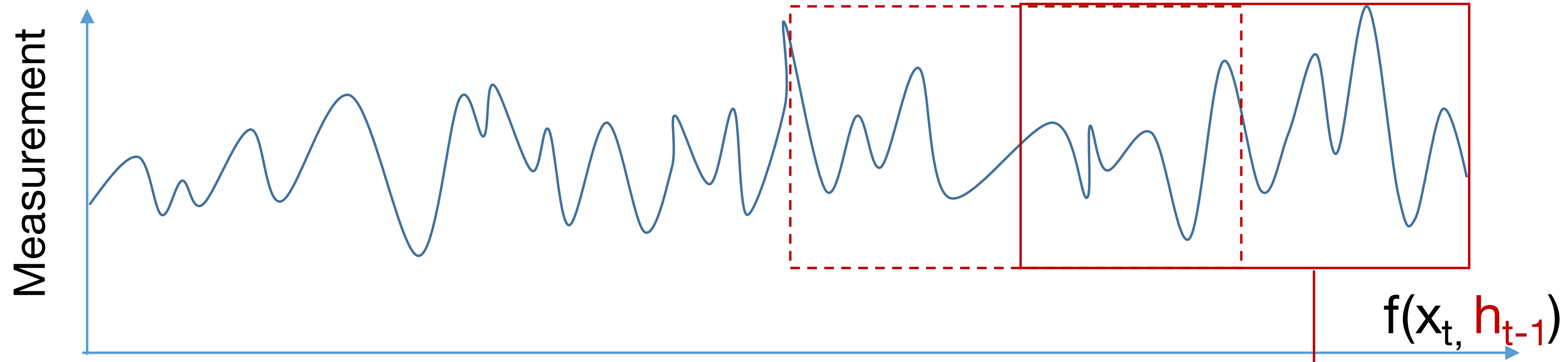
In [0]:
```
# another way to define models
# lets us access intermediate results too

mask_to_multiply = tf.Variable(initial_value = tf.initializers.GlorotNormal()(shape=(28,28,1)), trainable = True)
mask_to_multiply = tf.expand_dims(mask_to_multiply, 0) # add extra axis for batch size

#PHYSICAL LAYERS
input_image = tf.keras.layers.Input(shape = (28,28,1)) # Input layer, shape should be given as HWC
out = tf.math.multiply(input_image, mask_to_multiply) # hadamard product for illumination physical layer
out = tf.keras.layers.Conv2D(filters = 1, kernel_size = 5, strides =1, padding ="same", activation = "relu")(out) # con
##########################################################################################################################
```

Extensions beyond CNN's

Many-to-one recurrent neural network

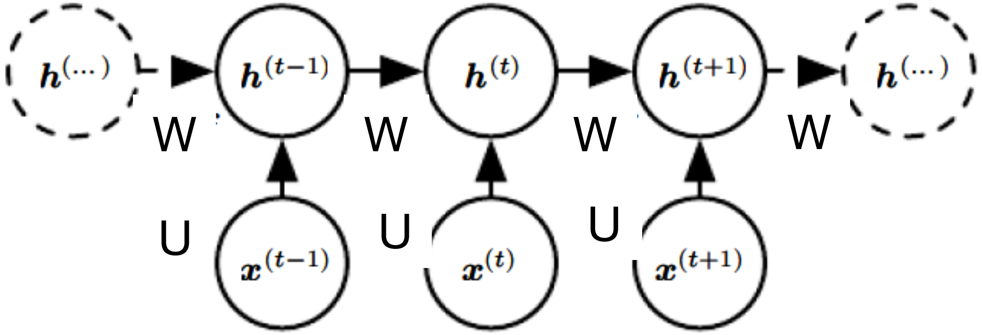


State h_t

$\boxed{V}$

Output o_t

Label y → Loss function $L(o_t, y)$



Backpropagate to minimize dL/dW, dL/DU

Simple network structure:

$$\boxed{h_t = \mathrm{ReLU}[\mathbf{W}h_{t-1} + \mathbf{U}x_t + b]}$$

The long short-term memory network

Forget gate:

$$f_i^{(t)} = \sigma \left(b_i^f + \sum_j U_{i,j}^f x_j^{(t)} + \sum_j W_{i,j}^f h_j^{(t-1)} \right)$$

Internal state:

$$s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma \left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right)$$

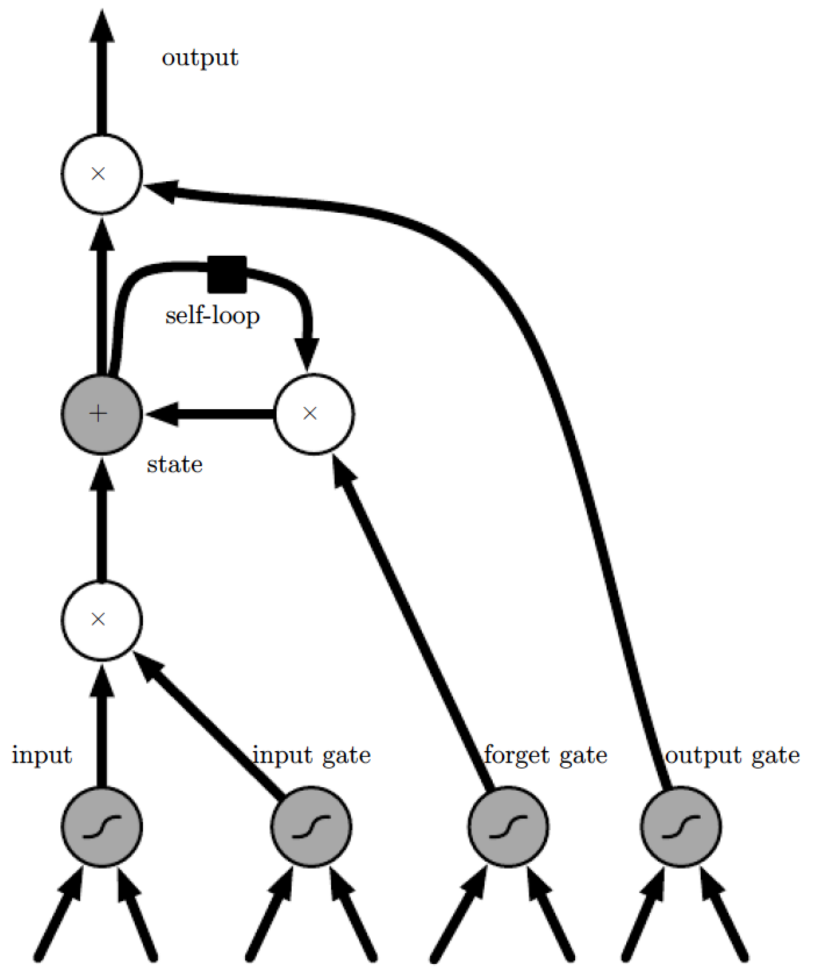
External input gate:

$$g_i^{(t)} = \sigma \left(b_i^g + \sum_j U_{i,j}^g x_j^{(t)} + \sum_j W_{i,j}^g h_j^{(t-1)} \right)$$

LSTM output:

$$h_i^{(t)} = \tanh \left(s_i^{(t)} \right) q_i^{(t)}$$

S. Hochreiter and J. Schmidhuber (1997)



Reinforcement learning - in a nutshell

- So far, we've looked at:
  1) Decisions from fixed images (classification, detection, segmentation)

CNN's

2) Decisions from time-sequence data (captioning as classification, etc.)

Decisions from images and time-sequence data (video classification, etc.)

RNN's

- Now, we're going to consider decisions for *dynamic data*
  - Most successful application: dynamic image data
    e.g.: video games, images of a Go game, car turning through obstacles

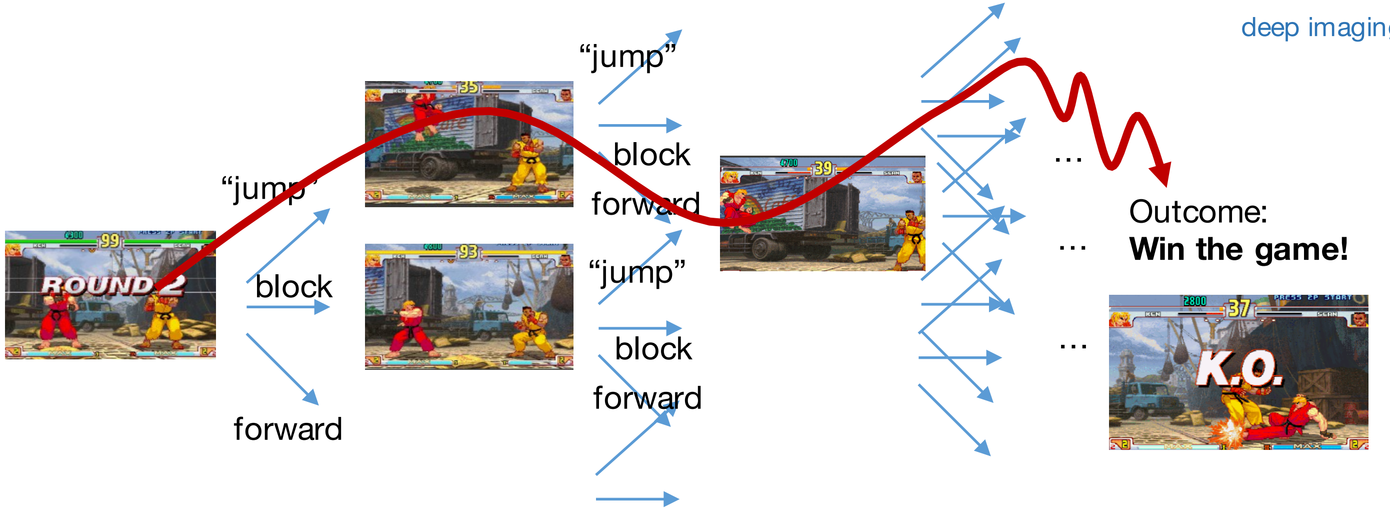
Reinforcement Learning

Supervised ML

Outcome:
Cell type B

- Fixed image sequence
- Goal: match to known label
  (large labeled dataset needed)
- Output: label
- Examines all data

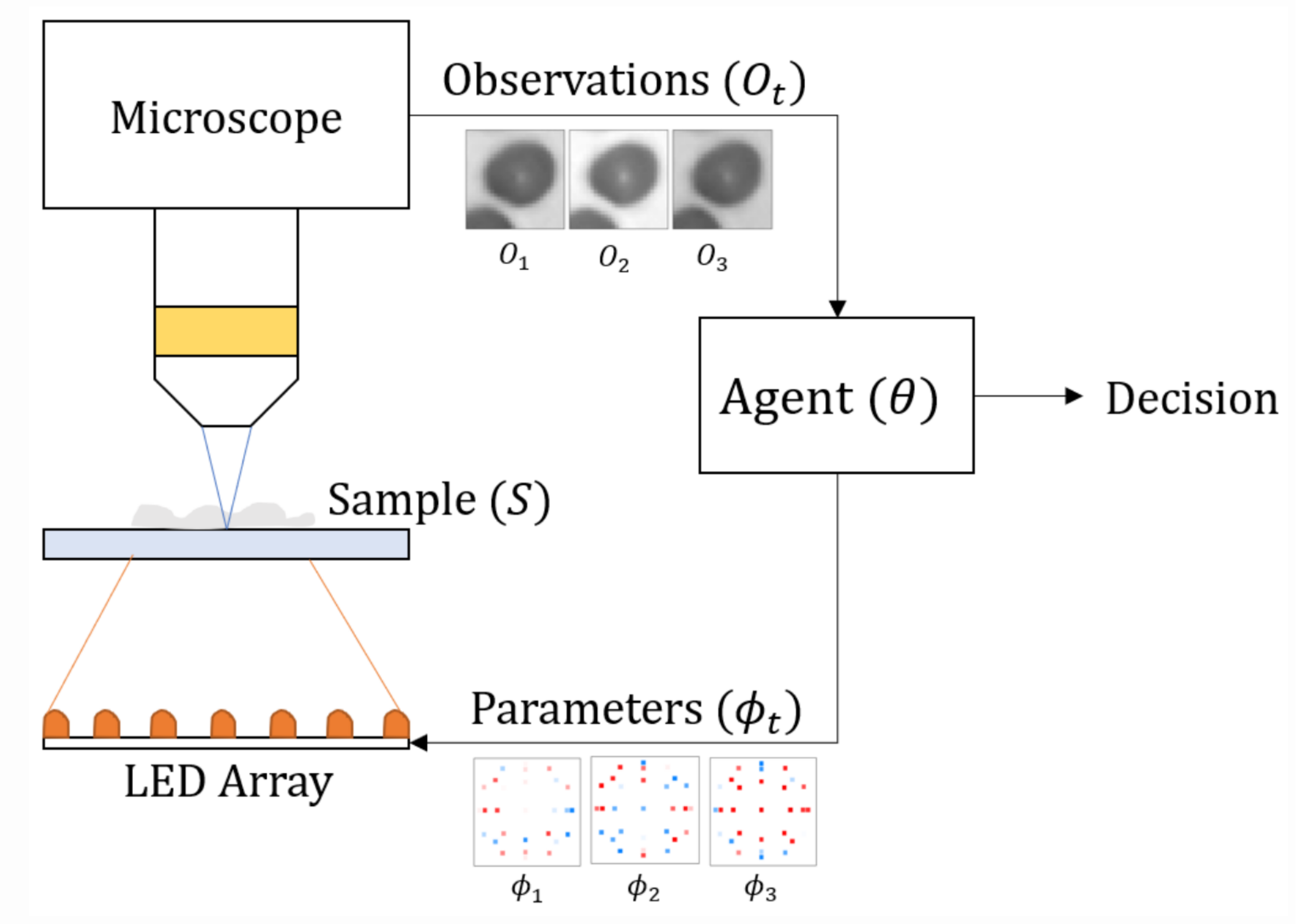
Reinforcement learning



Outcome:
Win the game!

- Dynamic image sequence
- Goal: get to known desired outcome
  (no labels needed, really…)
- Output: sequence of actions
- Not possible to examine *all* data

How can this be applied to optimized imaging?



deep imaging

The Machine Learning in Imaging Ethics Questionnaire

Situation 4: In 10 years, you go up to a modified microscope, "the Tissue Scanner 3000", that has a number of fancy lenses and lights. As a machine learning expert by now, you're aware that this microscope is optimized for looking at skin lesions. It performs a scan with a particular lighting configuration and reports a score of 98% confident that the lesion is benign, allowing you to look through other examples. It asks If you'd like another scan for additional confidence or a different outcome, at which point the illumination changes and it does some more scanning and reports a 99% confidence level. You can continue with another scan, but…

Are you now comfortable with leaving the office?

Yes:

No: