10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Backpropagation
+
Deep Learning

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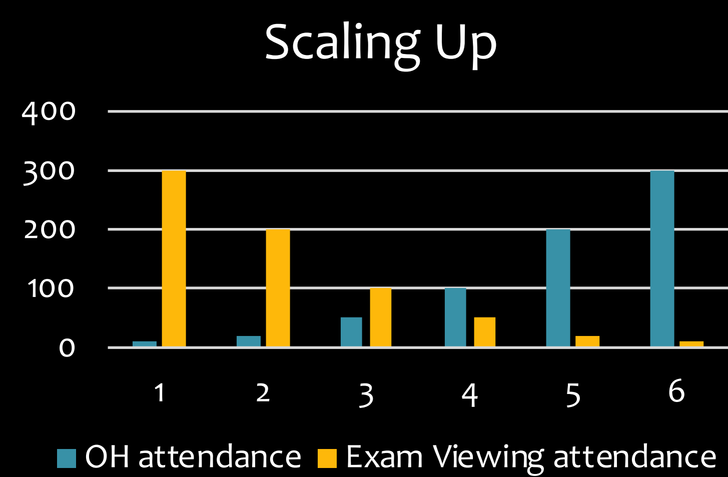
Lecture 14
Oct. 9, 2019

Reminders

- **Homework 4: Logistic Regression**
  - Out: Wed, Sep. 25
  - Due: Fri, Oct. 11 at 11:59pm
- **Homework 5: Neural Networks**
  - Out: Fri, Oct. 11
  - Due: Fri, Oct. 25 at 11:59pm
- **Today's In-Class Poll**
  - http://p14.mlcourse.org
- **Exam Viewing**



Q&A

Q: Do I need to know Matrix Calculus to derive the backprop algorithms used in this class?

A: No. We've carefully constructed our assignments so that you do **not** need to know Matrix Calculus.

That said, it's kind of handy.

Matrix Calculus

Let $y, x \in \mathbb{R}$ be scalars, $\mathbf{y} \in \mathbb{R}^M$ and $\mathbf{x} \in \mathbb{R}^P$ be vectors, and $\mathbf{Y} \in \mathbb{R}^{M \times N}$ and $\mathbf{X} \in \mathbb{R}^{P \times Q}$ be matrices

Numerator

Types of Derivatives	**scalar**	**vector**	**matrix**
scalar	$\frac{\partial y}{\partial x}$	$\frac{\partial \mathbf{y}}{\partial x}$	$\frac{\partial \mathbf{Y}}{\partial x}$
vector	$\frac{\partial y}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{Y}}{\partial \mathbf{x}}$
matrix	$\frac{\partial y}{\partial \mathbf{X}}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{X}}$	$\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}$

Denominator

Matrix Calculus

Types of Derivatives	**scalar**
scalar	$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x}\right]$
vector	$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix}$
matrix	$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial X_{11}} & \frac{\partial y}{\partial X_{12}} & \cdots & \frac{\partial y}{\partial X_{1Q}} \\ \frac{\partial y}{\partial X_{21}} & \frac{\partial y}{\partial X_{22}} & \cdots & \frac{\partial y}{\partial X_{2Q}} \\ \vdots & & & \vdots \\ \frac{\partial y}{\partial X_{P1}} & \frac{\partial y}{\partial X_{P2}} & \cdots & \frac{\partial y}{\partial X_{PQ}} \end{bmatrix}$

Matrix Calculus

Types of Derivatives	**scalar**	**vector**
scalar	$\frac{\partial y}{\partial x} = \begin{bmatrix} \frac{\partial y}{\partial x} \end{bmatrix}$	$\frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} & \frac{\partial y_2}{\partial x} & \cdots & \frac{\partial y_N}{\partial x} \end{bmatrix}$
vector	$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_N}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_N}{\partial x_2} \\ \vdots & & & \\ \frac{\partial y_1}{\partial x_P} & \frac{\partial y_2}{\partial x_P} & \cdots & \frac{\partial y_N}{\partial x_P} \end{bmatrix}$

Matrix Calculus

Common Vector Derivatives

Let $\frac{\partial f(\vec{x})}{\partial \vec{x}} = \nabla_x f(\vec{x})$ be the vector derivative of f, $B \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^m$

Scalar Derivative		Vector Derivative	
$f(x) \rightarrow \frac{\partial f}{\partial x}$		$f(x) \rightarrow \frac{\partial f}{\partial \vec{x}}$	
bx	$\rightarrow b$	$x^T B$	$\rightarrow B$
xb	$\rightarrow b$	$x^T b$	$\rightarrow b$
x^2	$\rightarrow 2x$	$x^T x$	$\rightarrow 2x$
bx^2	$\rightarrow 2bx$	$x^T B x$	$\rightarrow 2Bx$

B symmetric

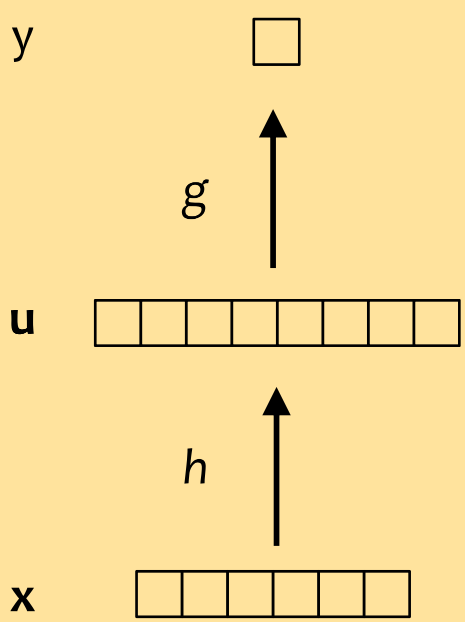
Matrix Calculus

Recall:

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix} \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \dots & \frac{\partial y_N}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_N}{\partial x_2} \\ \vdots & & & \\ \frac{\partial y_1}{\partial x_P} & \frac{\partial y_2}{\partial x_P} & \dots & \frac{\partial y_N}{\partial x_P} \end{bmatrix}$$

Question:

Suppose y = g(**u**) and **u** = h(**x**)



Which of the following is the correct definition of the chain rule?

Answer:

$$\frac{\partial y}{\partial \mathbf{x}} = \dots$$

A. $\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

B. $\frac{\partial y}{\partial \mathbf{u}}^T \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

C. $\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}^T$

D. $\frac{\partial y}{\partial \mathbf{u}}^T \frac{\partial \mathbf{u}}{\partial \mathbf{x}}^T$

E. $(\frac{\partial y}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}})^T$

F. None of the above

Algorithm

BACKPROPAGATION

Backpropagation

Chalkboard

– Example: Backpropagation for Chain Rule #1

Differentiation Quiz #1:

Suppose x = 2 and z = 3, what are dy/dx and dy/dz for the function below? **Round your answer to the nearest integer**.

$$y = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{xz}$$

Backprop Ex #1

$$y = f(x,z) = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{xz}$$

Forward Computation

Given $x=2$, $z=3$

$a = xz$

$b = \log(x)$

$c = \sin(b)$

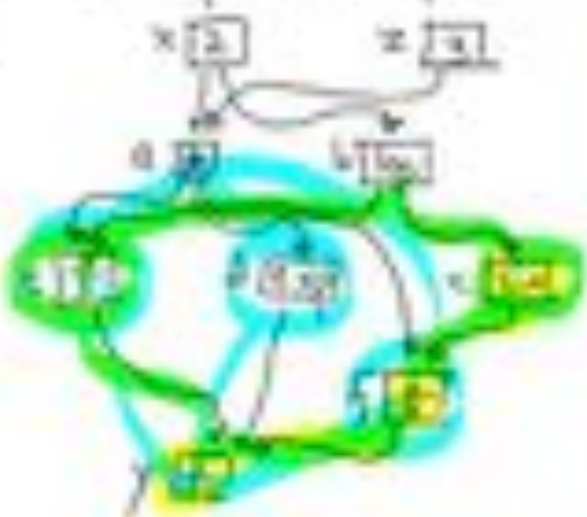
$d = \exp(a)$

$e = a/b$

$f = c/a$

$y = d+e+f$

Computation Graph



Backward Computation (aka Backprop)

$g_y = \frac{dy}{dy} = 1$

$g_d = \frac{dy}{dd} = 1$, $g_e = \frac{dy}{de} = 1$, $g_f = \frac{dy}{df} = 1$

$g_c = \frac{dy}{dc} = \frac{dy}{df}\frac{df}{dc} = g_f\left(\frac{1}{a}\right)$

$g_b = \frac{dy}{db} = \frac{dy}{de}\frac{de}{db} + \frac{dy}{dc}\frac{dc}{db}$

$= g_e\left(-\frac{a}{b^2}\right) + g_c(\cos(b))$

$g_a = \frac{dy}{da} = \frac{dy}{de}\frac{de}{da} + \frac{dy}{dd}\frac{dd}{da} + \frac{dy}{df}\frac{df}{da}$

$= g_e\left(\frac{1}{b}\right) + g_d(\exp(a)) + g_f\left(-\frac{c}{a^2}\right)$

$g_x = g_a(z) + g_b\left(\frac{1}{x}\right)$

Updates:

$$g_x = \frac{dy}{dx} = \sum_{k=1}^{K} \underbrace{\frac{dy}{du_k}}_{g_{u_k}}\frac{du_k}{dx}$$

Backpropagation

Chalkboard

- SGD for Neural Network
- Example: Backpropagation for Neural Network

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

<u>Forward Computation</u>

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph"**)
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1,\ldots, v_N$
   a. Compute $u_i = g_i(v_1,\ldots, v_N)$
   b. Store the result at the node

<u>Backward Computation (Version A)</u>

1. **Initialize** $dy/dy = 1$.
2. Visit each node v_j in **reverse topological order**.
   Let $u_1,\ldots, u_M$ denote all the nodes with v_j as an input
   Assuming that $y = h(\mathbf{u}) = h(u_1,\ldots, u_M)$
   and $\mathbf{u} = g(\mathbf{v})$ or equivalently $u_i = g_i(v_1,\ldots, v_j,\ldots, v_N)$ for all i
   a. We already know dy/du_i for all i
   b. Compute dy/dv_j as below (Choice of algorithm ensures computing (du_i/dv_j) is easy)

$$\frac{dy}{dv_j} = \sum_{i=1}^{M} \frac{dy}{du_i}\frac{du_i}{dv_j}$$

Return partial derivatives dy/du_i for all variables

Training

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1, \ldots, v_N$
   a. Compute $u_i = g_i(v_1, \ldots, v_N)$
   b. Store the result at the node

Backward Computation (Version B)

1. **Initialize** all partial derivatives dy/du_j to 0 and $dy/dy = 1$.
2. Visit each node in **reverse topological order**.
   For variable $u_i = g_i(v_1, \ldots, v_N)$
   a. We already know dy/du_i
   b. Increment dy/dv_j by $(dy/du_i)(du_i/dv_j)$
   (Choice of algorithm ensures computing (du_i/dv_j) is easy)

Return partial derivatives dy/du_i for all variables

Backpropagation

Why is the backpropagation algorithm efficient?

1. Reuses **computation from the forward pass** in the backward pass
2. Reuses **partial derivatives** throughout the backward pass (*but only if the algorithm reuses shared computation in the forward pass*)

   (Key idea: partial derivatives in the backward pass should be thought of as variables stored for reuse)

Training — SGD with Backprop

Example: 1-Hidden Layer Neural Network

Algorithm 1 Stochastic Gradient Descent (SGD)

procedure SGD(Training data $\mathcal{D}$, test data $\mathcal{D}_t$)
  Initialize parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$
  for $e \in \{1, 2, \ldots, E\}$ **do**
    for $(\mathbf{x}, \mathbf{y}) \in \mathcal{D}$ **do**
      Compute neural network layers:
      $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{b}, \mathbf{z}, \hat{\mathbf{y}}, J) = \text{NNFORWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta})$
      Compute gradients via backprop:
      $\left.\begin{array}{l} \mathbf{g}_{\boldsymbol{\alpha}} = \nabla_{\boldsymbol{\alpha}} J \\ \mathbf{g}_{\boldsymbol{\beta}} = \nabla_{\boldsymbol{\beta}} J \end{array}\right\} = \text{NNBACKWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{o})$
      Update parameters:
      $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \gamma \mathbf{g}_{\boldsymbol{\alpha}}$
      $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \gamma \mathbf{g}_{\boldsymbol{\beta}}$
    Evaluate training mean cross-entropy $J_{\mathcal{D}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
    Evaluate test mean cross-entropy $J_{\mathcal{D}_t}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
  return parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$

Backpropagation

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

Forward

$J = cos(u)$

$u = u_1 + u_2$

$u_1 = sin(t)$

$u_2 = 3t$

$t = x^2$

Training

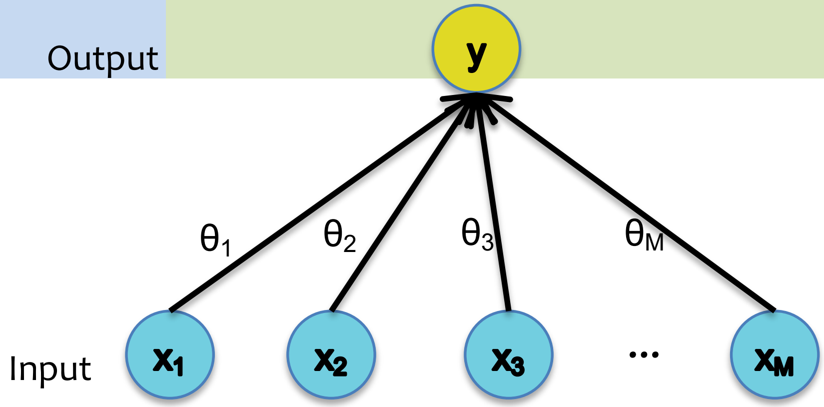
Backpropagation

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

Forward	Backward
$J = cos(u)$	$\frac{dJ}{du}$ += $-sin(u)$
$u = u_1 + u_2$	$\frac{dJ}{du_1}$ += $\frac{dJ}{du}\frac{du}{du_1}, \quad \frac{du}{du_1} = 1$ $\quad$ $\frac{dJ}{du_2}$ += $\frac{dJ}{du}\frac{du}{du_2}, \quad \frac{du}{du_2} = 1$
$u_1 = sin(t)$	$\frac{dJ}{dt}$ += $\frac{dJ}{du_1}\frac{du_1}{dt}, \quad \frac{du_1}{dt} = \cos(t)$
$u_2 = 3t$	$\frac{dJ}{dt}$ += $\frac{dJ}{du_2}\frac{du_2}{dt}, \quad \frac{du_2}{dt} = 3$
$t = x^2$	$\frac{dJ}{dx}$ += $\frac{dJ}{dt}\frac{dt}{dx}, \quad \frac{dt}{dx} = 2x$

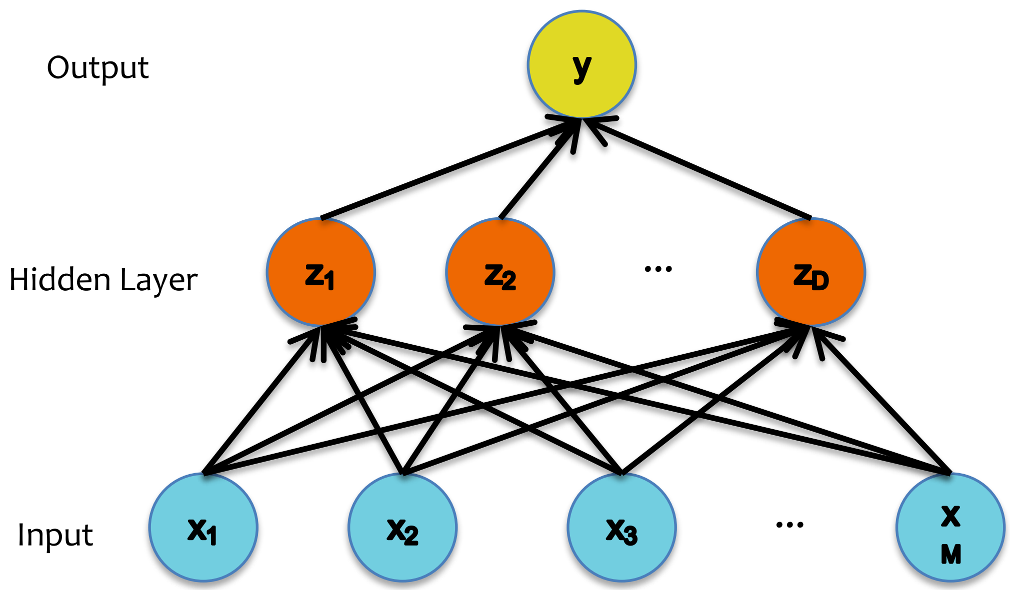
Training Backpropagation

Case 1: Logistic Regression



Forward	Backward
$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
$y = \frac{1}{1 + \exp(-a)}$	$\frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da}, \quad \frac{dy}{da} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$
$a = \sum_{j=0}^{D} \theta_j x_j$	$\frac{dJ}{d\theta_j} = \frac{dJ}{da}\frac{da}{d\theta_j}, \quad \frac{da}{d\theta_j} = x_j$ $\frac{dJ}{dx_j} = \frac{dJ}{da}\frac{da}{dx_j}, \quad \frac{da}{dx_j} = \theta_j$

Training | Backpropagation



(E) **Output (sigmoid)**
$$y = \frac{1}{1+\exp(-b)}$$

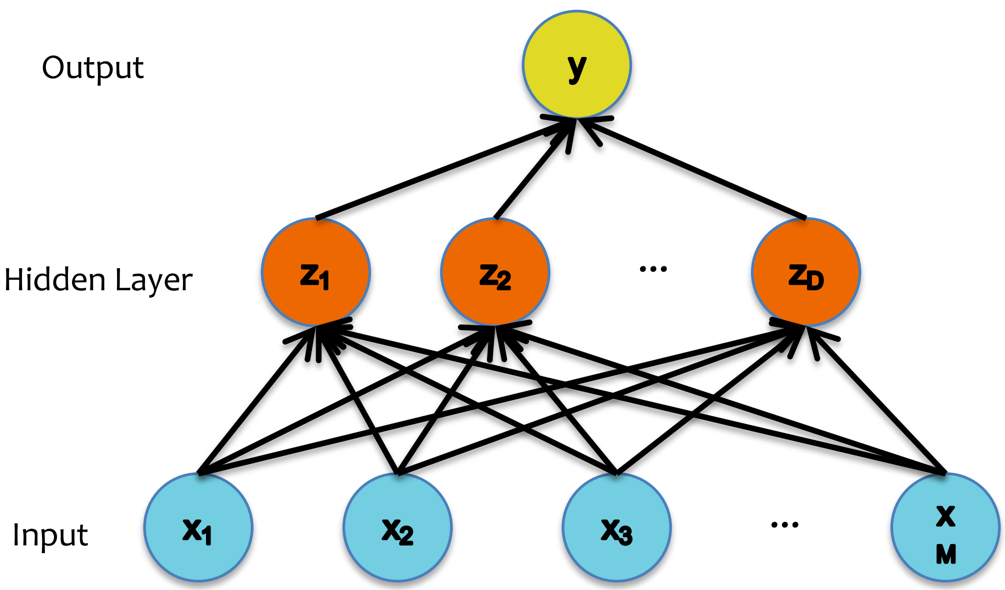
(D) **Output (linear)**
$$b = \sum_{j=0}^{D} \beta_j z_j$$

(C) **Hidden (sigmoid)**
$$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$$

(B) **Hidden (linear)**
$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$$

(A) **Input**
Given $x_i, \ \forall i$

Training | Backpropagation



(F) Loss
$J = \frac{1}{2}(y - y^*)^2$

↑

(E) Output (sigmoid)
$y = \frac{1}{1+\exp(-b)}$

↑

(D) Output (linear)
$b = \sum_{j=0}^{D} \beta_j z_j$

↑

(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

↑

(B) Hidden (linear)
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

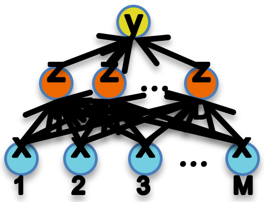
↑

(A) Input
Given $x_i, \ \forall i$

Training

Backpropagation

Case 2: Neural Network



Forward

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

$$y = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$$

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$$

$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$$

$$\frac{dJ}{dx_i} = \sum_{j=0}^{D} \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \alpha_{ji}$$

Training Backpropagation

Case 2:

	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$ $\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$ $\frac{dJ}{dx_i} = \sum_{j=0}^{D} \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \alpha_{ji}$

Derivative of a Sigmoid

First suppose that

$$s = \frac{1}{1 + \exp(-b)} \tag{1}$$

To obtain the simplified form of the derivative of a sigmoid.

$$\begin{align}
\frac{ds}{db} &= \frac{\exp(-b)}{(\exp(-b) + 1)^2} \tag{2} \\
&= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1 + 1 - 1)^2} \tag{3} \\
&= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1)^2} \tag{4} \\
&= \frac{\exp(-b) + 1}{(\exp(-b) + 1)^2} - \frac{1}{(\exp(-b) + 1)^2} \tag{5} \\
&= \frac{1}{(\exp(-b) + 1)} - \frac{1}{(\exp(-b) + 1)^2} \tag{6} \\
&= \frac{1}{(\exp(-b) + 1)} - \left(\frac{1}{(\exp(-b) + 1)} \frac{1}{(\exp(-b) + 1)}\right) \tag{7} \\
&= \frac{1}{(\exp(-b) + 1)} \left(1 - \frac{1}{(\exp(-b) + 1)}\right) \tag{8} \\
&= s(1 - s) \tag{9}
\end{align}$$

Training Backpropagation

Case 2:

	Forward	Backward
Loss	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Sigmoid	$y = \frac{1}{1 + \exp(-b)}$	$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \boxed{\frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}}$
Linear	$b = \sum_{j=0}^{D} \beta_j z_j$	$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \frac{db}{d\beta_j} = z_j$ $\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \frac{db}{dz_j} = \beta_j$
Sigmoid	$z_j = \frac{1}{1 + \exp(-a_j)}$	$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \boxed{\frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}}$
Linear	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \frac{da_j}{d\alpha_{ji}} = x_i$ $\frac{dJ}{dx_i} = \sum_{j=0}^{D} \frac{dJ}{da_j}\frac{da_j}{dx_i}, \frac{da_j}{dx_i} = \alpha_{ji}$

Training | Backpropagation

Case 2:

	Forward	Backward
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Training

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1, \ldots, v_N$
   a. Compute $u_i = g_i(v_1, \ldots, v_N)$
   b. Store the result at the node

Backward Computation (Version A)

1. **Initialize** $dy/dy = 1$.
2. Visit each node v_j in **reverse topological order**.
   Let $u_1, \ldots, u_M$ denote all the nodes with v_j as an input
   Assuming that $y = h(\mathbf{u}) = h(u_1, \ldots, u_M)$
   and $\mathbf{u} = g(\mathbf{v})$ or equivalently $u_i = g_i(v_1, \ldots, v_j, \ldots, v_N)$ for all i
   a. We already know dy/du_i for all i
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$$\frac{dy}{dv_j} = \sum_{i=1}^{M} \frac{dy}{du_i} \frac{du_i}{dv_j}$$

Return partial derivatives dy/du_i for all variables

Training

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

<u>Forward Computation</u>

1. Write an **algorithm** for evaluating the function y = f(**x**). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1, \ldots, v_N$
   a. Compute $u_i = g_i(v_1, \ldots, v_N)$
   b. Store the result at the node

<u>Backward Computation (Version B)</u>

1. **Initialize** all partial derivatives dy/du_j to 0 and $dy/dy = 1$.
2. Visit each node in **reverse topological order**.
   For variable $u_i = g_i(v_1, \ldots, v_N)$
   a. We already know dy/du_i
   b. Increment dy/dv_j by $(dy/du_i)(du_i/dv_j)$
   (Choice of algorithm ensures computing (du_i/dv_j) is easy)

Return partial derivatives dy/du_i for all variables

Training

SGD with Backprop

Example: 1-Hidden Layer Neural Network

Algorithm 1 Stochastic Gradient Descent (SGD)

procedure SGD(Training data $\mathcal{D}$, test data $\mathcal{D}_t$)
  Initialize parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$
  for $e \in \{1, 2, \ldots, E\}$ **do**
    for $(\mathbf{x}, \mathbf{y}) \in \mathcal{D}$ **do**
      Compute neural network layers:
      $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{b}, \mathbf{z}, \hat{\mathbf{y}}, J) = \text{NNFORWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta})$
      Compute gradients via backprop:
      $$\left.\begin{array}{l} \mathbf{g}_{\boldsymbol{\alpha}} = \nabla_{\boldsymbol{\alpha}} J \\ \mathbf{g}_{\boldsymbol{\beta}} = \nabla_{\boldsymbol{\beta}} J \end{array}\right\} = \text{NNBACKWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{o})$$
      Update parameters:
      $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \gamma \mathbf{g}_{\boldsymbol{\alpha}}$
      $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \gamma \mathbf{g}_{\boldsymbol{\beta}}$
    Evaluate training mean cross-entropy $J_{\mathcal{D}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
    Evaluate test mean cross-entropy $J_{\mathcal{D}_t}(\boldsymbol{\alpha}, \boldsymbol{\beta})$
  return parameters $\boldsymbol{\alpha}, \boldsymbol{\beta}$

Background

A Recipe for

Gradients

Backpropagation can compute this gradient!

And it's a **special case of a more general algorithm** called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of th

– Decision functio

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

$\boldsymbol{y}_i)$

opposite the gradient)

$$\boldsymbol{\theta}^{(t} \quad {}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

OTHER APPROACHES TO DIFFERENTIATION

Training

Finite Difference Method

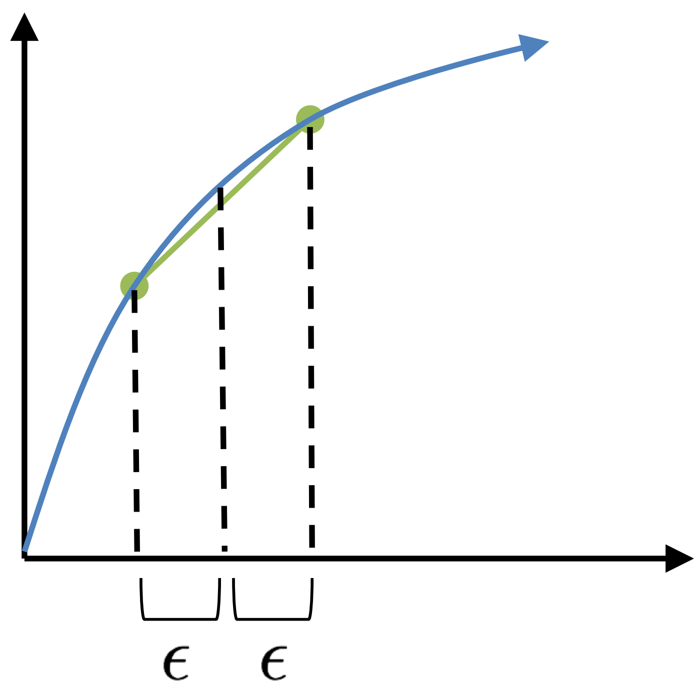
The *centered* finite difference approximation is:

$$\frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta}) \approx \frac{(J(\boldsymbol{\theta} + \epsilon \cdot \boldsymbol{d}_i) - J(\boldsymbol{\theta} - \epsilon \cdot \boldsymbol{d}_i))}{2\epsilon} \quad (1)$$

where $\boldsymbol{d}_i$ is a 1-hot vector consisting of all zeros except for the ith entry of $\boldsymbol{d}_i$, which has value 1.

Notes:

- Suffers from issues of floating point precision, in practice
- Typically only appropriate to use on small examples with an appropriately chosen epsilon



Symbolic Differentiation

Speed Quiz:
2 minute time limit.

Differentiation Quiz #1:

Suppose x = 2 and z = 3, what are dy/dx and dy/dz for the function below? **Round your answer to the nearest integer**.

$$y = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{xz}$$

Answer: *Answers below are in the form [dy/dx, dy/dz]*

A. [42, -72]
B. [72, -42]
C. [100, 127]
D. [127, 100]
E. [1208, 810]
F. [810, 1208]
G. [1505, 94]
H. [94, 1505]

Symbolic Differentiation

Differentiation Quiz #2:

A neural network with 2 hidden layers can be written as:

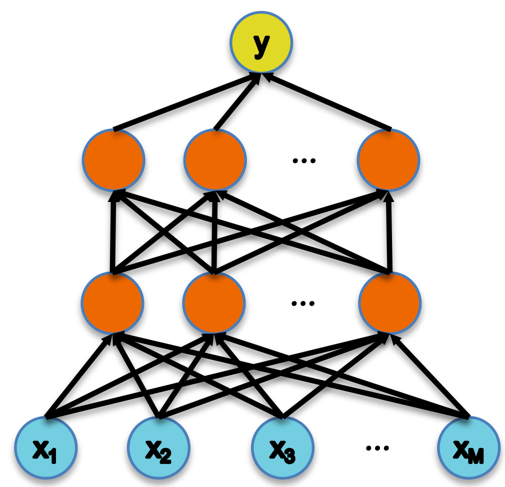
$$y = \sigma(\boldsymbol{\beta}^T \sigma((\boldsymbol{\alpha}^{(2)})^T \sigma((\boldsymbol{\alpha}^{(1)})^T \mathbf{x}))$$

where $y \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^{D^{(0)}}$, $\boldsymbol{\beta} \in \mathbb{R}^{D^{(2)}}$ and $\boldsymbol{\alpha}^{(i)}$ is a $D^{(i)} \times D^{(i-1)}$ matrix. Nonlinear functions are applied elementwise:

$$\sigma(\mathbf{a}) = [\sigma(a_1), \ldots, \sigma(a_K)]^T$$

Let σ be sigmoid: $\sigma(a) = \frac{1}{1+exp{-a}}$

What is $\frac{\partial y}{\partial \beta_j}$ and $\frac{\partial y}{\partial \alpha_j^{(i)}}$ for all i, j.



Summary

1. **Neural Networks…**
   - provide a way of learning features
   - are highly nonlinear prediction functions
   - (can be) a highly parallel network of logistic regression classifiers
   - discover useful hidden representations of the input
2. **Backpropagation…**
   - provides an efficient way to compute gradients
   - is a special case of reverse-mode automatic differentiation

Backprop Objectives

You should be able to…

- Construct a computation graph for a function as specified by an algorithm
- Carry out the backpropagation on an arbitrary computation graph
- Construct a computation graph for a neural network, identifying all the given and intermediate quantities that are relevant
- Instantiate the backpropagation algorithm for a neural network
- Instantiate an optimization method (e.g. SGD) and a regularizer (e.g. L2) when the parameters of a model are comprised of several matrices corresponding to different layers of a neural network
- Apply the empirical risk minimization framework to learn a neural network
- Use the finite difference method to evaluate the gradient of a function
- Identify when the gradient of a function can be computed at all and when it can be computed efficiently

DEEP LEARNING

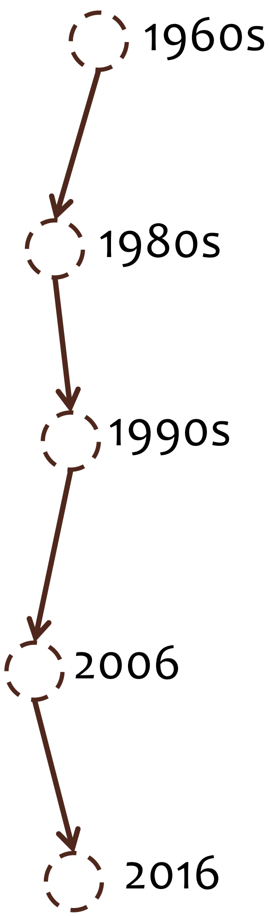
Deep Learning Outline

- **Background: Computer Vision**
  - Image Classification
  - ILSVRC 2010 - 2016
  - Traditional Feature Extraction Methods
  - Convolution as Feature Extraction
- **Convolutional Neural Networks (CNNs)**
  - Learning Feature Abstractions
  - Common CNN Layers:
    - Convolutional Layer
    - Max-Pooling Layer
    - Fully-connected Layer (w/tensor input)
    - Softmax Layer
    - ReLU Layer
  - Background: Subgradient
  - Architecture: LeNet
  - Architecture: AlexNet
- **Training a CNN**
  - SGD for CNNs
  - Backpropagation for CNNs

Why is everyone talking about Deep Learning?

- Because a lot of money is invested in it…
  - DeepMind: Acquired by Google for **$400 million**
  - DNNResearch: **Three person startup** (including Geoff Hinton) acquired by Google for unknown price tag
  - Enlitic, Ersatz, MetaMind, Nervana, Skylab: Deep Learning startups commanding **millions of VC dollars**
- Because it made the **front page** of the New York Times

Why is everyone talking about Deep Learning?



Deep learning:

- Has won numerous pattern recognition competitions
- Does so with minimal feature engineering

This wasn't always the case!

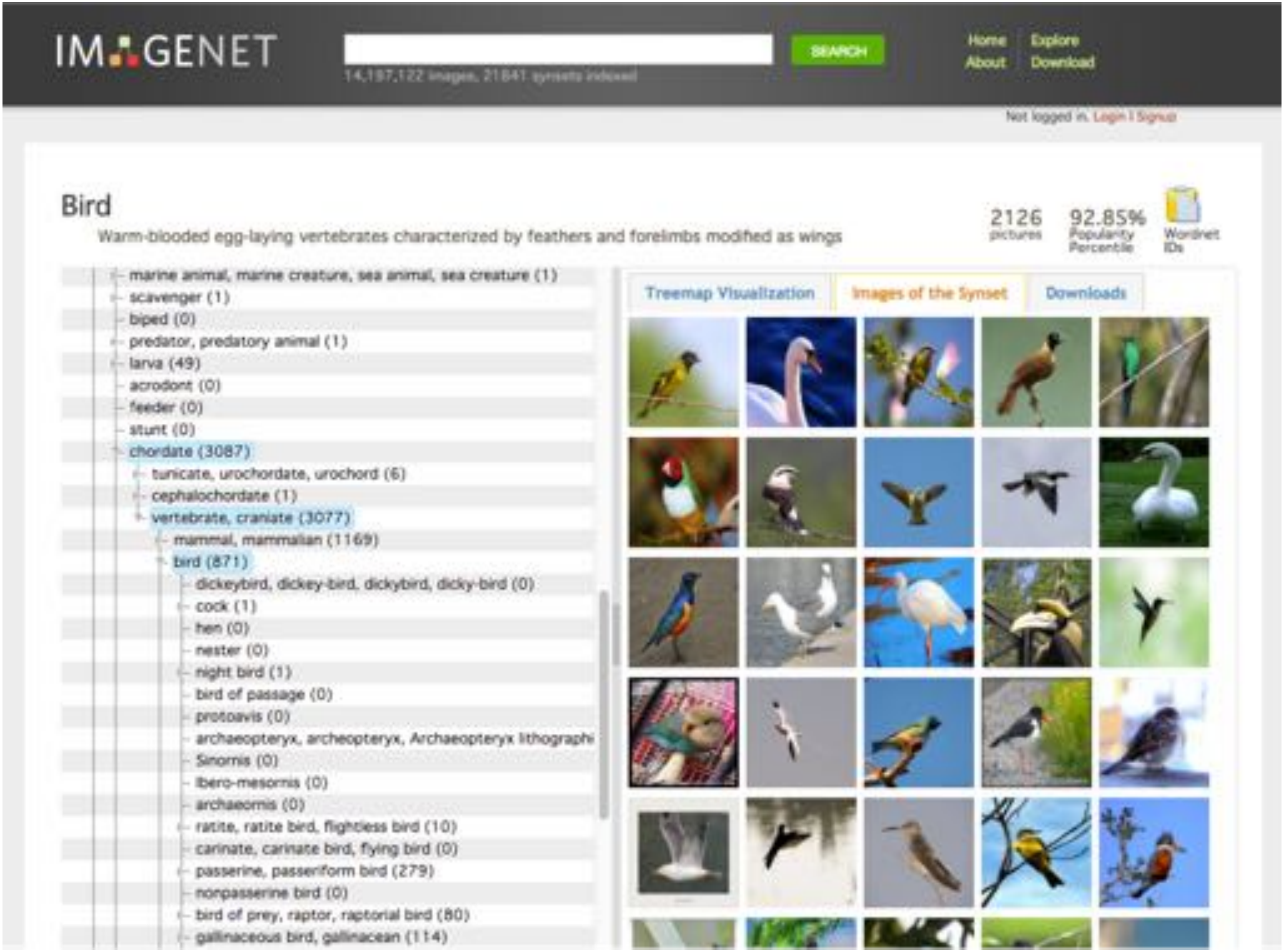
Since 1980s: Form of models hasn't changed much, but lots of new tricks…

- More hidden units
- Better (online) optimization
- New nonlinear functions (ReLUs)
- Faster computers (CPUs and GPUs)

BACKGROUND: COMPUTER VISION

Example: Image Classification

- ImageNet LSVRC-2011 contest:
  - **Dataset:** 1.2 million labeled images, 1000 classes
  - **Task**: Given a new image, label it with the correct class
  - **Multiclass** classification problem
- Examples from http://image-net.org/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14,197,122 images, 21841 synsets indexed
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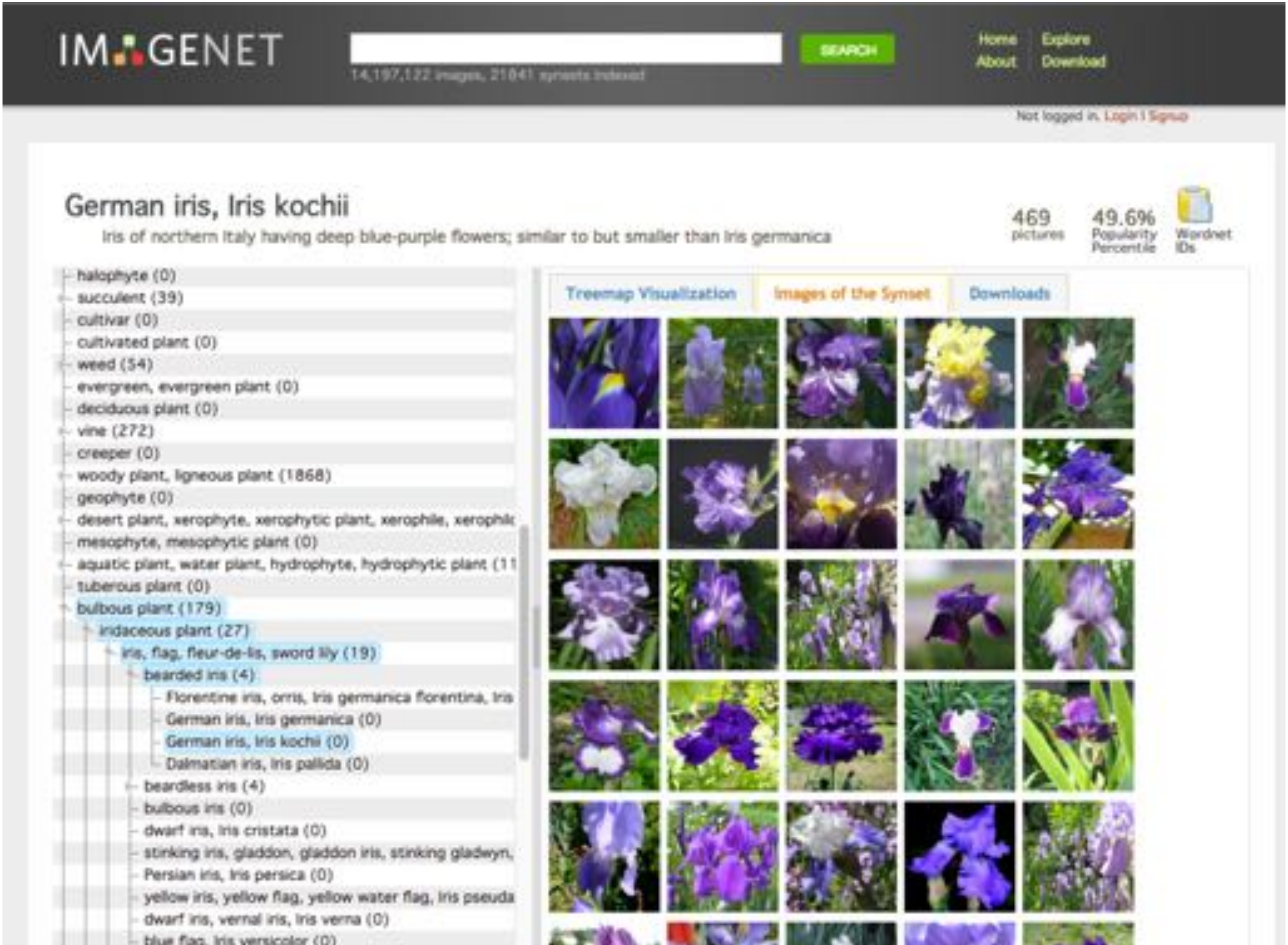
Bird
Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings
2126
pictures
92.85%
Popularity Percentile
Wordnet IDs
marine animal, marine creature, sea animal, sea creature (1)
scavenger (1)
biped (0)
predator, predatory animal (1)
larva (49)
acrodont (0)
feeder (0)
stunt (0)
chordate (3087)
tunicate, urochordate, urochord (6)
cephalochordate (1)
vertebrate, craniate (3077)
mammal, mammalian (1169)
bird (871)
dickeybird, dickey-bird, dickybird, dicky-bird (0)
cock (1)
hen (0)
nester (0)
night bird (1)
bird of passage (0)
protoavis (0)
archaeopteryx, archeopteryx, Archaeopteryx lithographi
Sinornis (0)
Ibero-mesornis (0)
archaeornis (0)
ratite, ratite bird, flightless bird (10)
carinate, carinate bird, flying bird (0)
passerine, passeriform bird (279)
nonpasserine bird (0)
bird of prey, raptor, raptorial bird (80)
gallinaceous bird, gallinacean (114)
Treemap Visualization
Images of the Synset
Downloads



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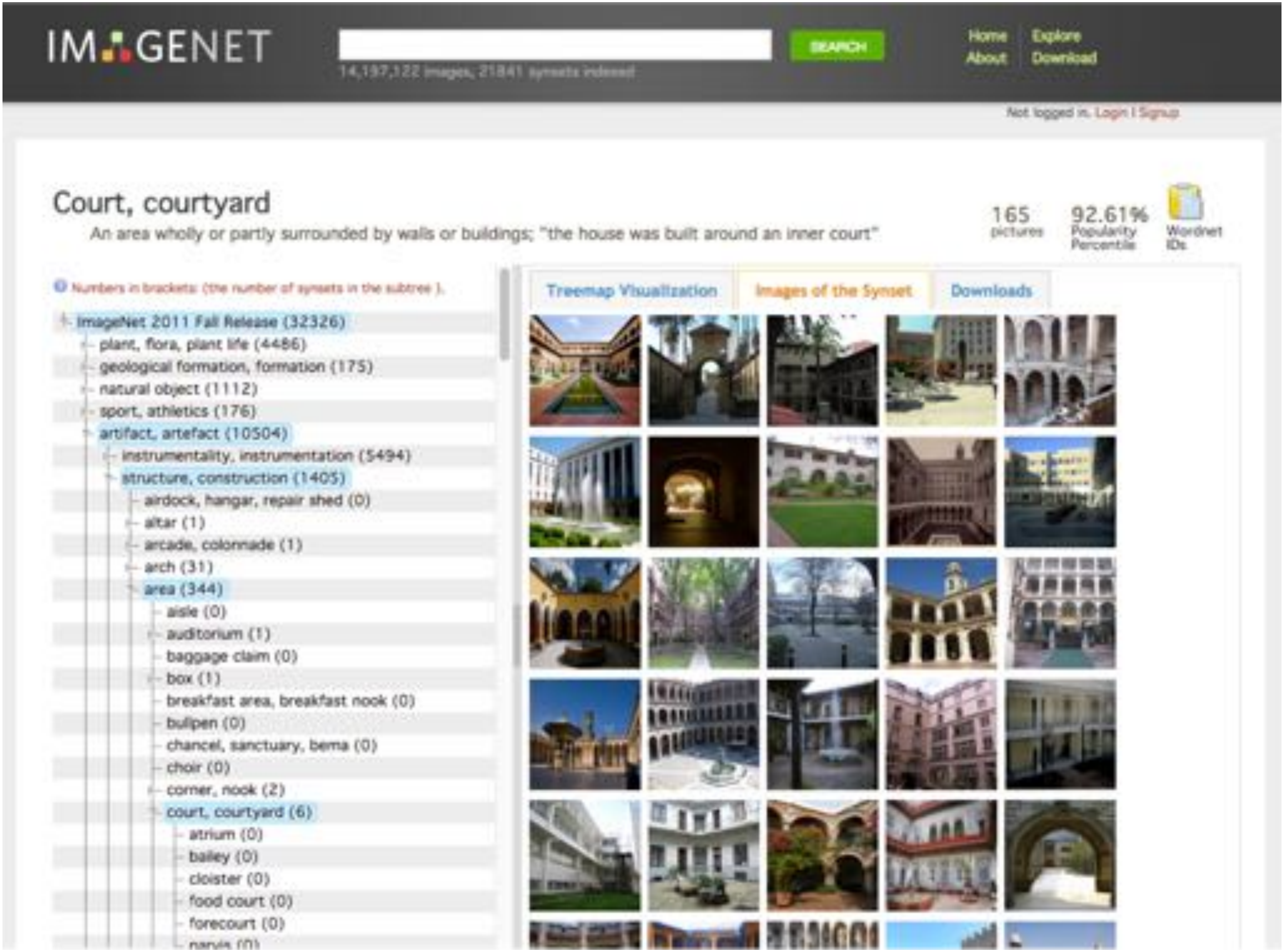
German iris, Iris kochii
Iris of northern Italy having deep blue-purple flowers; similar to but smaller than Iris germanica
469
pictures
49.6%
Popularity Percentile
Wordnet IDs
halophyte (0)
succulent (39)
cultivar (0)
cultivated plant (0)
weed (54)
evergreen, evergreen plant (0)
deciduous plant (0)
vine (272)
creeper (0)
woody plant, ligneous plant (1868)
geophyte (0)
desert plant, xerophyte, xerophytic plant, xerophile, xerophilc
mesophyte, mesophytic plant (0)
aquatic plant, water plant, hydrophyte, hydrophytic plant (11
tuberous plant (0)
bulbous plant (179)
iridaceous plant (27)
iris, flag, fleur-de-lis, sword lily (19)
bearded iris (4)
Florentine iris, orris, Iris germanica florentina, Iris
German iris, Iris germanica (0)
German iris, Iris kochii (0)
Dalmatian iris, Iris pallida (0)
beardless iris (4)
bulbous iris (0)
dwarf iris, Iris cristata (0)
stinking iris, gladdon, gladdon iris, stinking gladwyn,
Persian iris, Iris persica (0)
yellow iris, yellow flag, yellow water flag, Iris pseuda
dwarf iris, vernal iris, Iris verna (0)
blue flag, Iris versicolor (0)
Treemap Visualization
Images of the Synset
Downloads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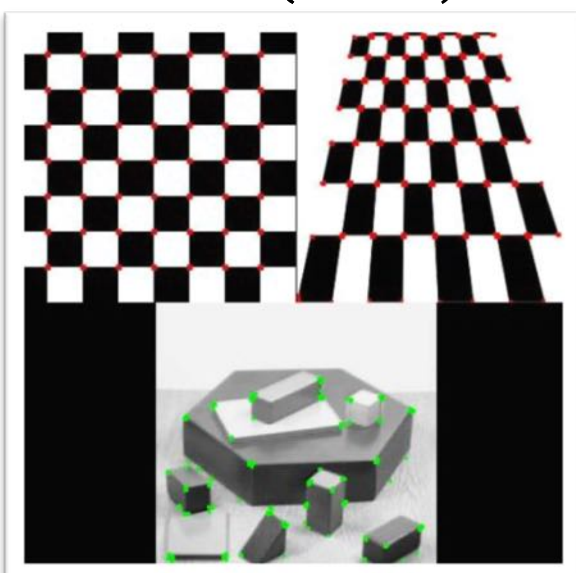
Court, courtyard
An area wholly or partly surrounded by walls or buildings; "the house was built around an inner court"
165
pictures
92.61%
Popularity
Percentile
Wordnet
IDs
Numbers in brackets: (the number of synsets in the subtree).
ImageNet 2011 Fall Release (32326)
plant, flora, plant life (4486)
geological formation, formation (175)
natural object (1112)
sport, athletics (176)
artifact, artefact (10504)
instrumentality, instrumentation (5494)
structure, construction (1405)
airdock, hangar, repair shed (0)
altar (1)
arcade, colonnade (1)
arch (31)
area (344)
aisle (0)
auditorium (1)
baggage claim (0)
box (1)
breakfast area, breakfast nook (0)
bullpen (0)
chancel, sanctuary, bema (0)
choir (0)
corner, nook (2)
court, courtyard (6)
atrium (0)
bailey (0)
cloister (0)
food court (0)
forecourt (0)
Treemap Visualization
Images of the Synset
Downloads

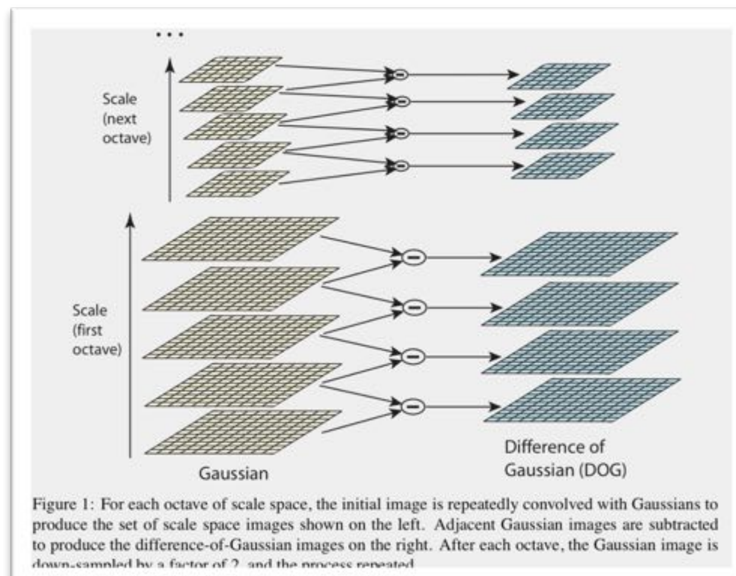
Feature Engineering for CV

Edge detection (Canny)

Corner Detection (Harris)



Scale Invariant Feature Transform (SIFT)



Figures from http://opencv.org

Figure from Lowe (1999) and Lowe (2004)

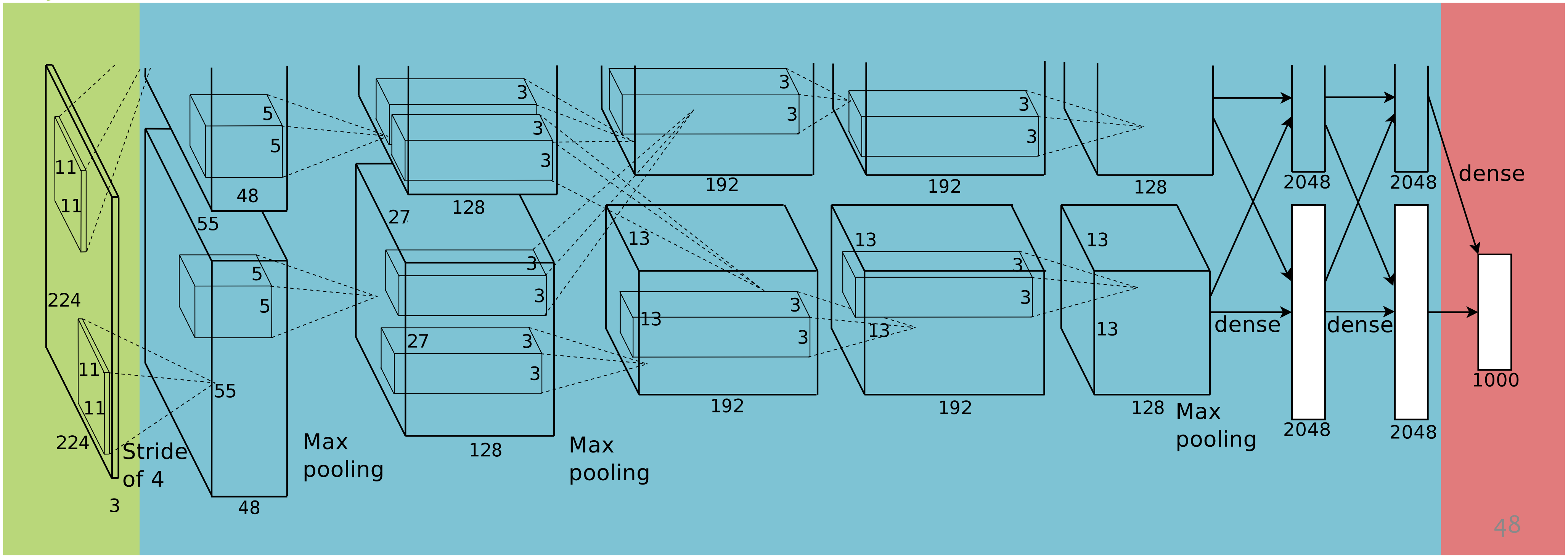
Example: Image Classification

CNN for Image Classification
(Krizhevsky, Sutskever & Hinton, 2012)
15.3% error on ImageNet LSVRC-2012 contest

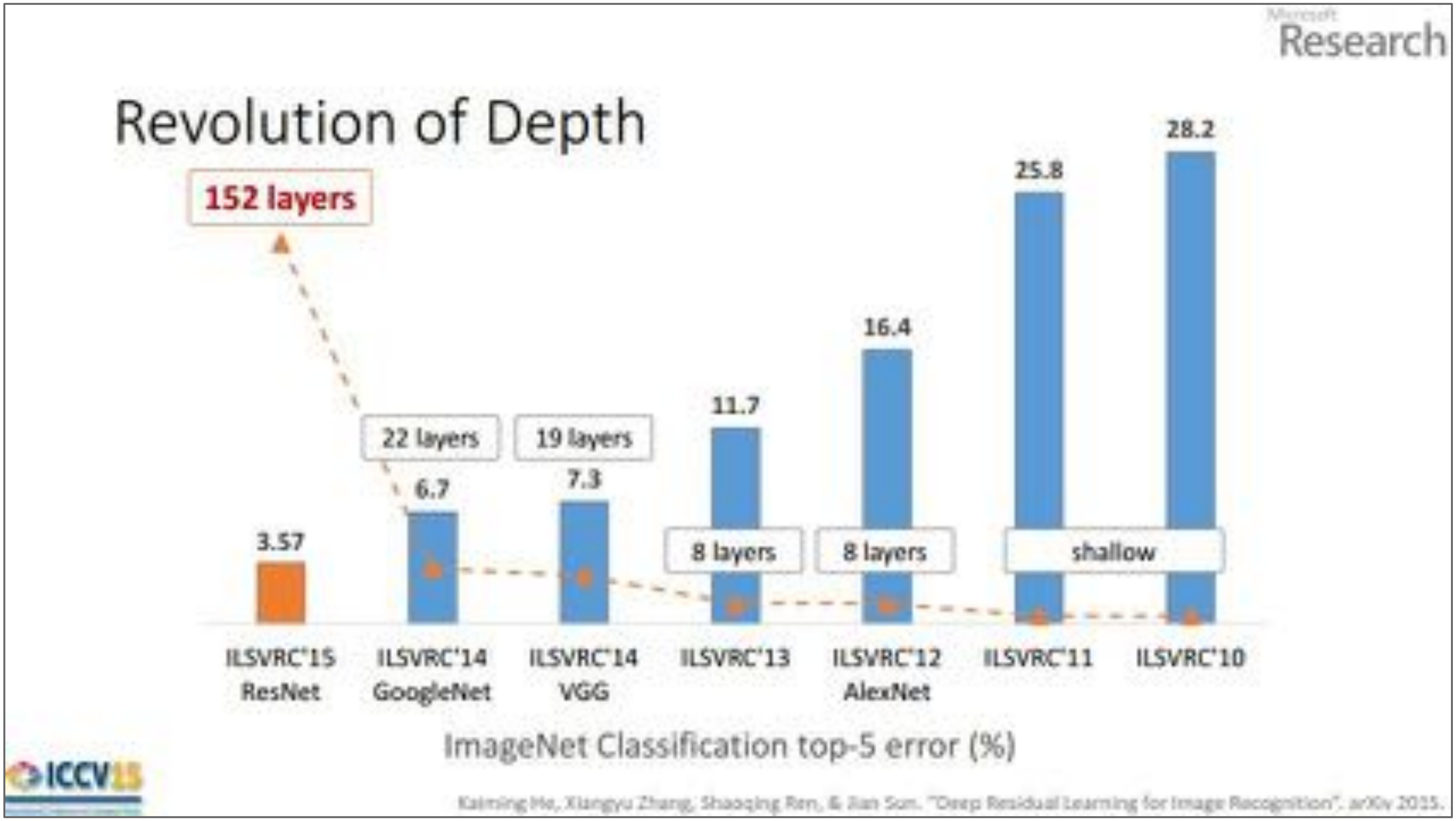
Input image (pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

1000-way softmax



CNNs for Image Recognition



Slide from Kaiming He

CONVOLUTION

What’s a convolution?

- Basic idea:
  - Pick a 3x3 matrix F of weights
  - Slide this over an image and compute the “inner product” (similarity) of F and the corresponding field of the image, and replace the pixel in the center of the field with the output of the inner product operation
- Key point:
  - Different convolutions extract different types of low-level “features” from an image
  - All that we need to vary to generate these different features is the weights of F

Ex: 1 input channel, 1 output channel

$$\underset{\text{Input}}{\begin{array}{|c|c|c|}\hline x_{11} & x_{12} & x_{13} \\ \hline x_{21} & x_{22} & x_{23} \\ \hline x_{31} & x_{32} & x_{33} \\ \hline\end{array}} \longrightarrow \underset{\text{Conv}}{\begin{array}{|c|c|}\hline \alpha_{11} & \alpha_{12} \\ \hline \alpha_{21} & \alpha_{22} \\ \hline\end{array}} \longrightarrow \underset{\text{Output}}{\begin{array}{|c|c|}\hline y_{11} & y_{12} \\ \hline y_{21} & y_{22} \\ \hline\end{array}}$$

$$y_{11} = \alpha_{11} x_{11} + \alpha_{12} x_{12} + \alpha_{21} x_{21} + \alpha_{22} x_{22} + \alpha_0$$

$$y_{12} = \alpha_{11} x_{12} + \alpha_{12} x_{13} + \alpha_{21} x_{22} + \alpha_{22} x_{23} + \alpha_0$$

$$y_{21} = \alpha_{11} x_{21} + \alpha_{12} x_{22} + \alpha_{21} x_{31} + \alpha_{22} x_{32} + \alpha_0$$

$$y_{22} = \alpha_{11} x_{22} + \alpha_{12} x_{23} + \alpha_{21} x_{32} + \alpha_{22} x_{33} + \alpha_0$$

Slide adapted from William Cohen

Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution

0	0	0
0	1	1
0	1	0

Convolved Image

1	1	1	1	1
1	0	0	1	0
1	0	1	0	0
1	1	0	0	0
1	0	0	0	0

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Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution

0	0	0
0	1	1
0	1	0

Convolved Image

3	2	2	3	1
2	0	2	1	0
2	2	1	0	0
3	1	0	0	0
1	0	0	0	0

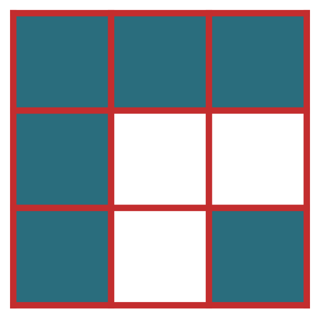
Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution



Convolved Image

3	2	2	3	1
2	0	2	1	0
2	2	1	0	0
3	1	0	0	0
1	0	0	0	0

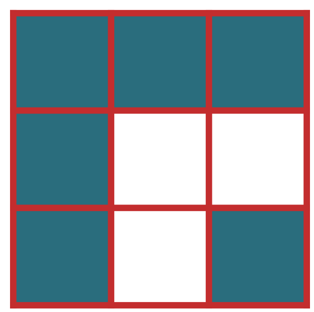
Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution



Convolved Image

3	2	2	3	1
2	0	2	1	0
2	2	1	0	0
3	1	0	0	0
1	0	0	0	0

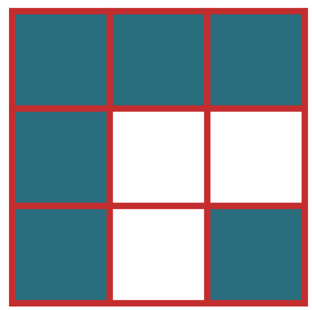
Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution

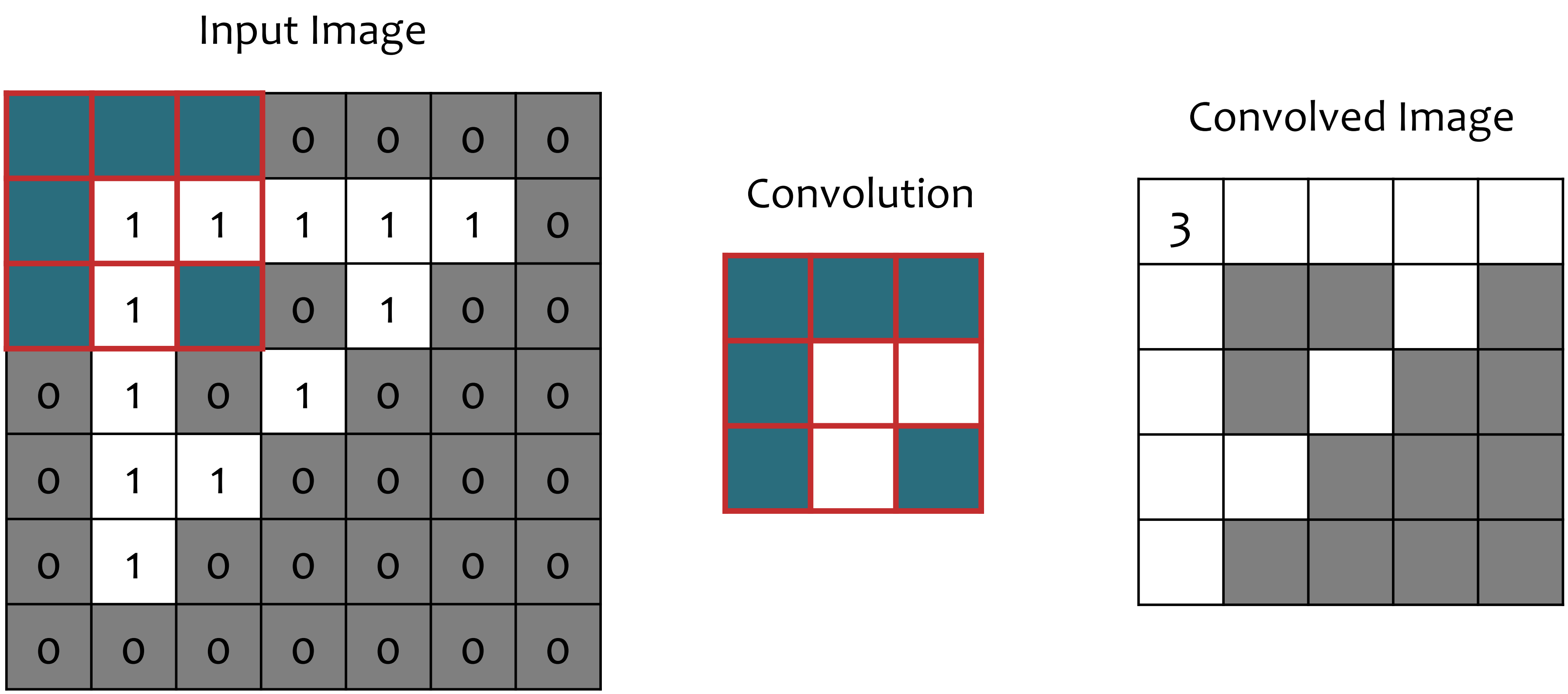


Convolved Image

3	2	2	3	1
2	0	2	1	0
2	2	1	0	0
3	1	0	0	0
1	0	0	0	0

Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.



Background: Image Processing

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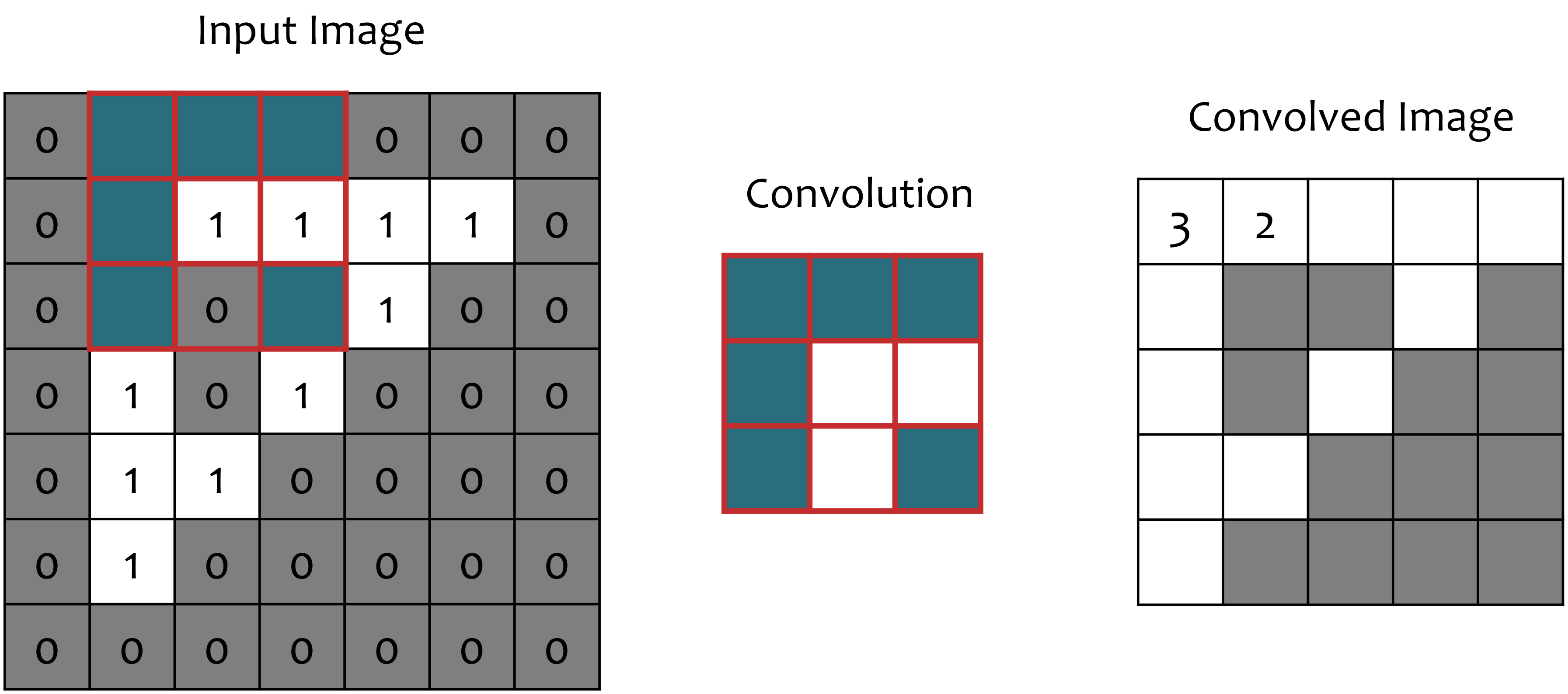

Background: Image Processing

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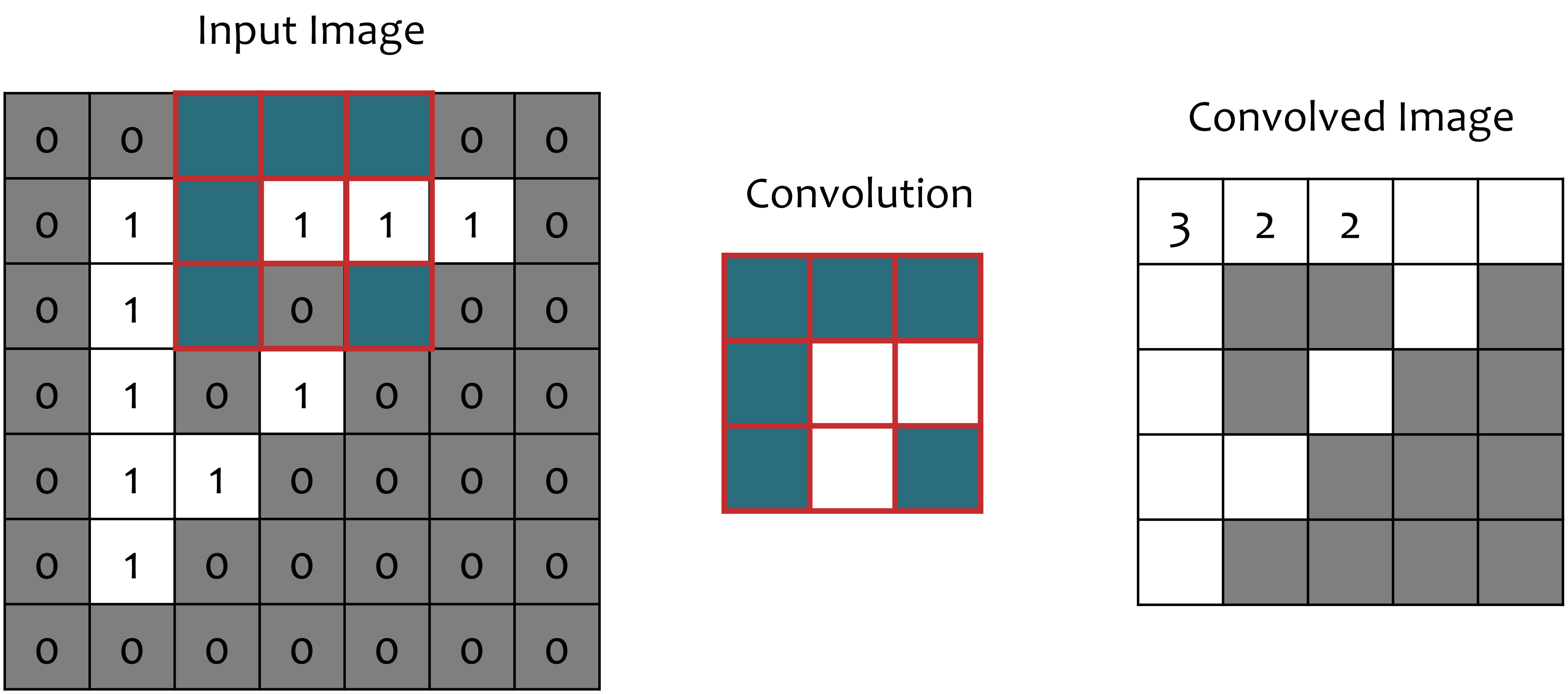

Background: Image Processing

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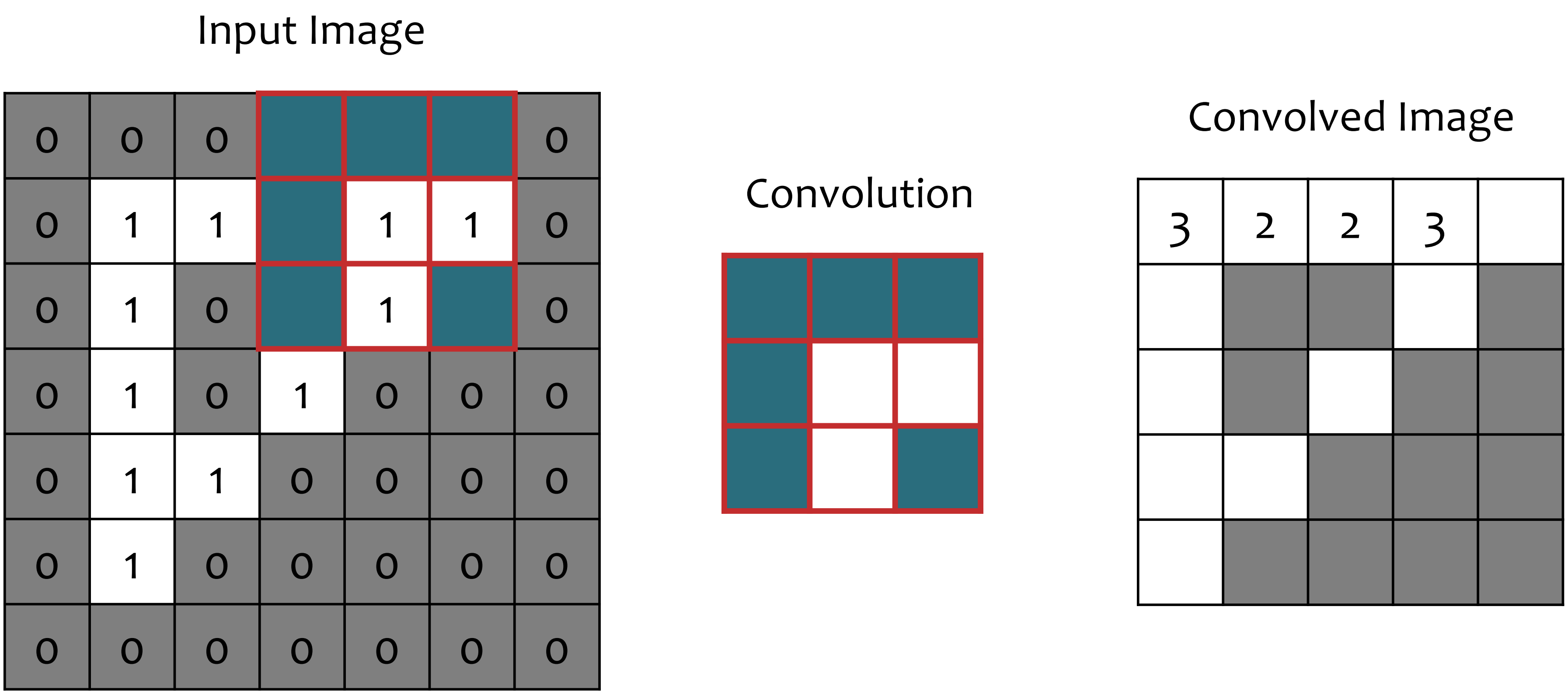

Background: Image Processing

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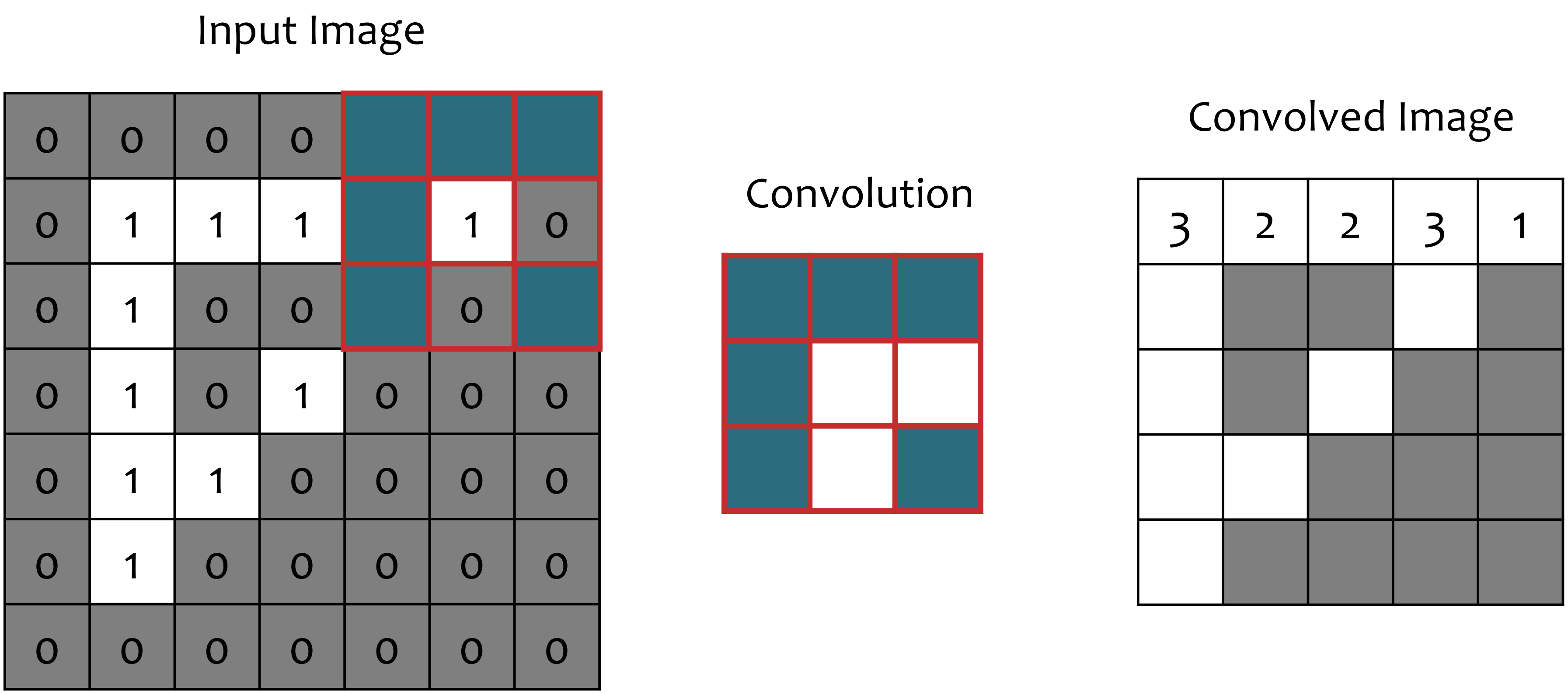

Background: Image Processing

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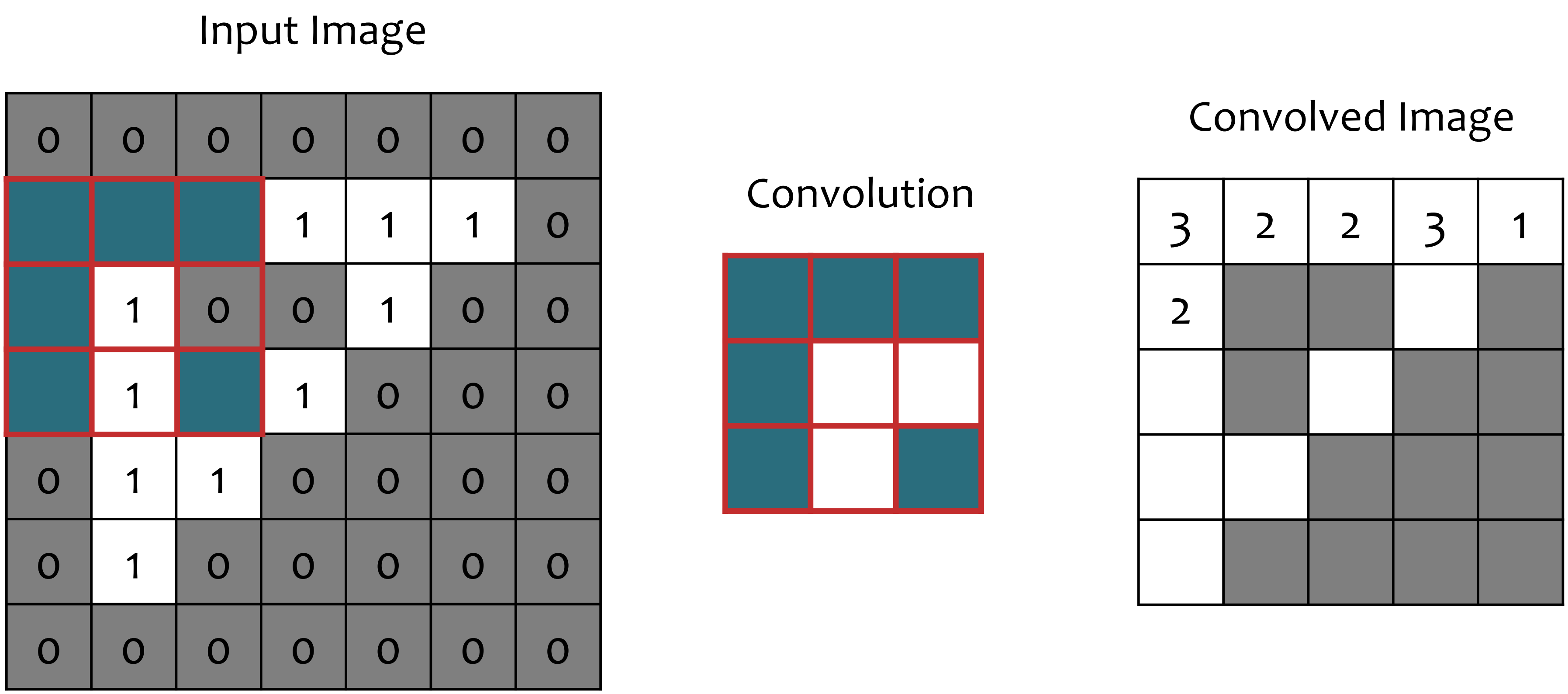
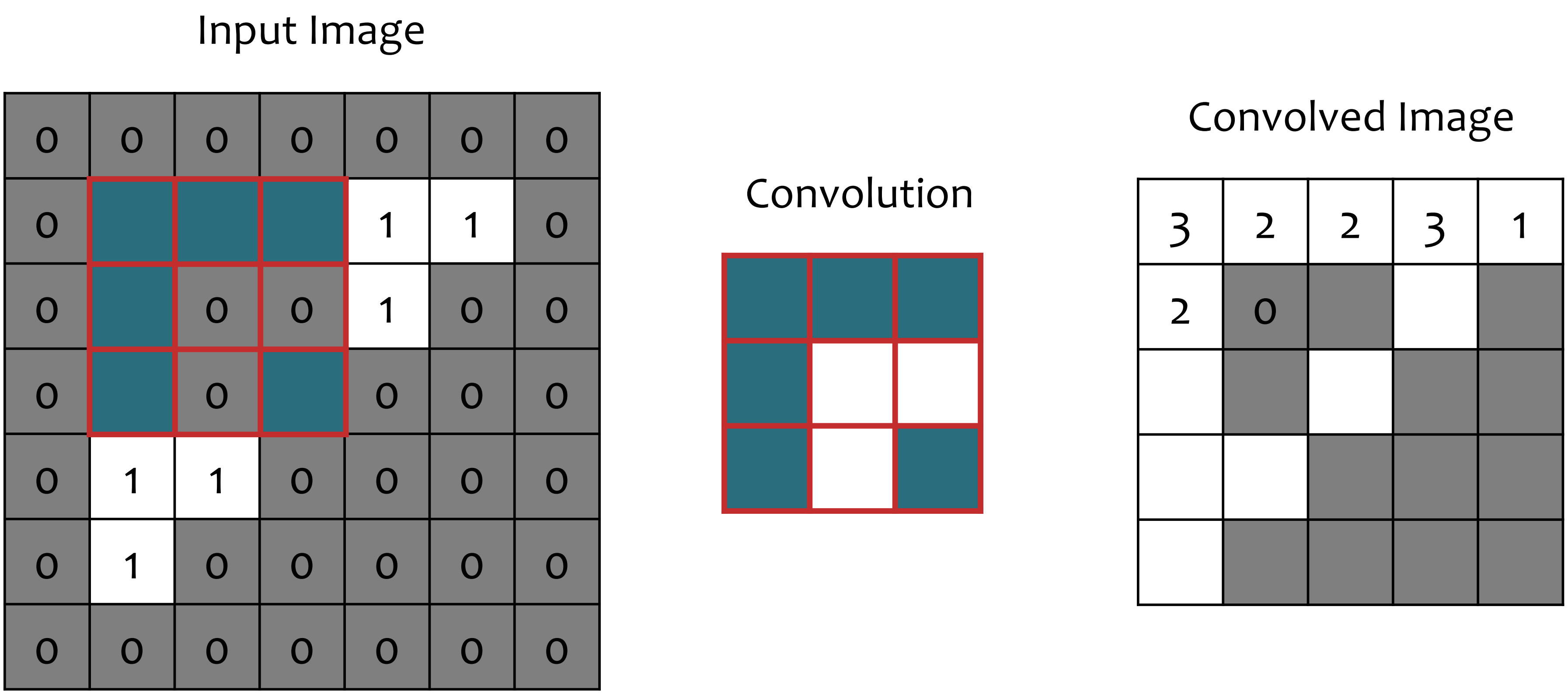


Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.



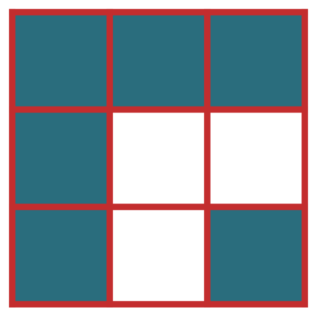
Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Convolution



Convolved Image

3	2	2	3	1
2	0	2	1	0
2	2	1	0	0
3	1	0	0	0
1	0	0	0	0

Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Identity Convolution

0	0	0
0	1	0
0	0	0

Convolved Image

1	1	1	1	1
1	0	0	1	0
1	0	1	0	0
1	1	0	0	0
1	0	0	0	0

Background: Image Processing

A **convolution matrix** is used in image processing for tasks such as edge detection, blurring, sharpening, etc.

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Blurring Convolution

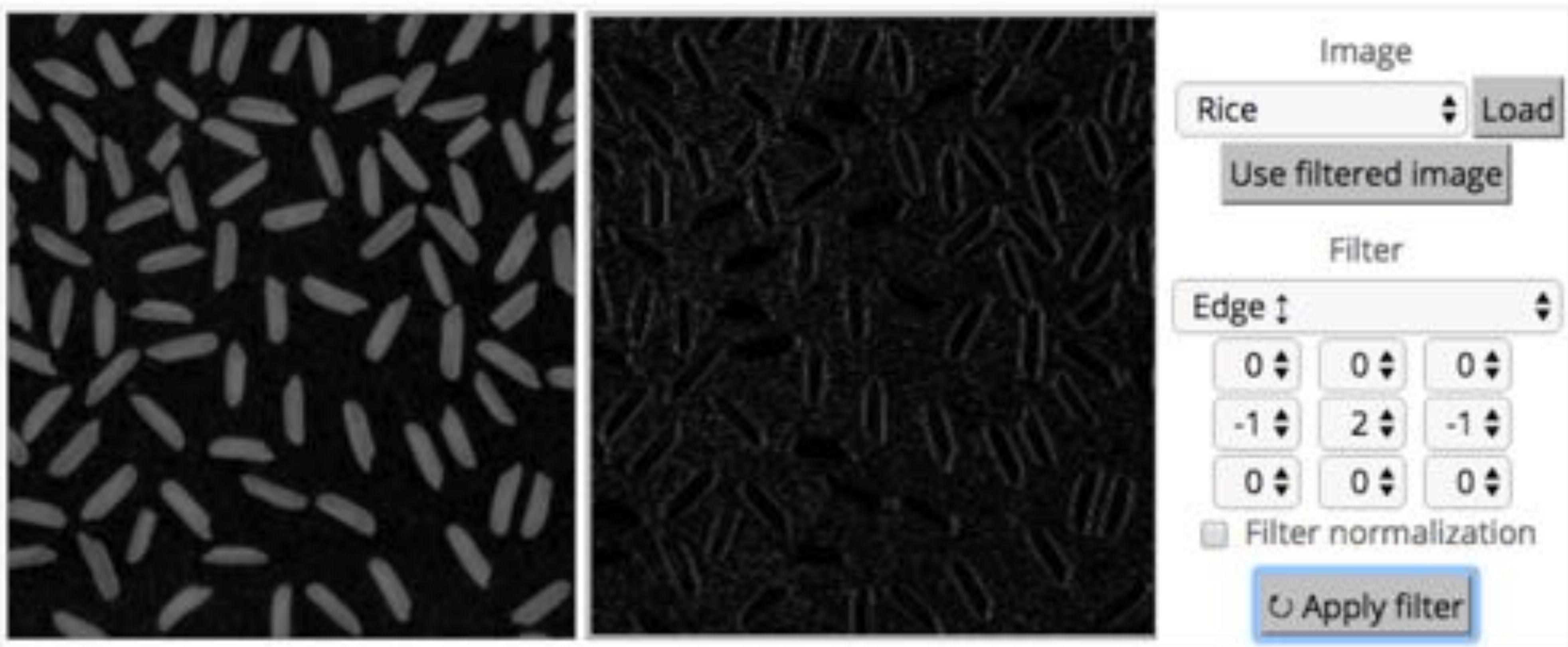
.1	.1	.1
.1	.2	.1
.1	.1	.1

Convolved Image

.4	.5	.5	.5	.4
.4	.2	.3	.6	.3
.5	.4	.4	.2	.1
.5	.6	.2	.1	0
.4	.3	.1	0	0

What’s a convolution?

http://matlabtricks.com/post-5/3x3-convolution-kernels-with-online-demo



Slide from William Cohen

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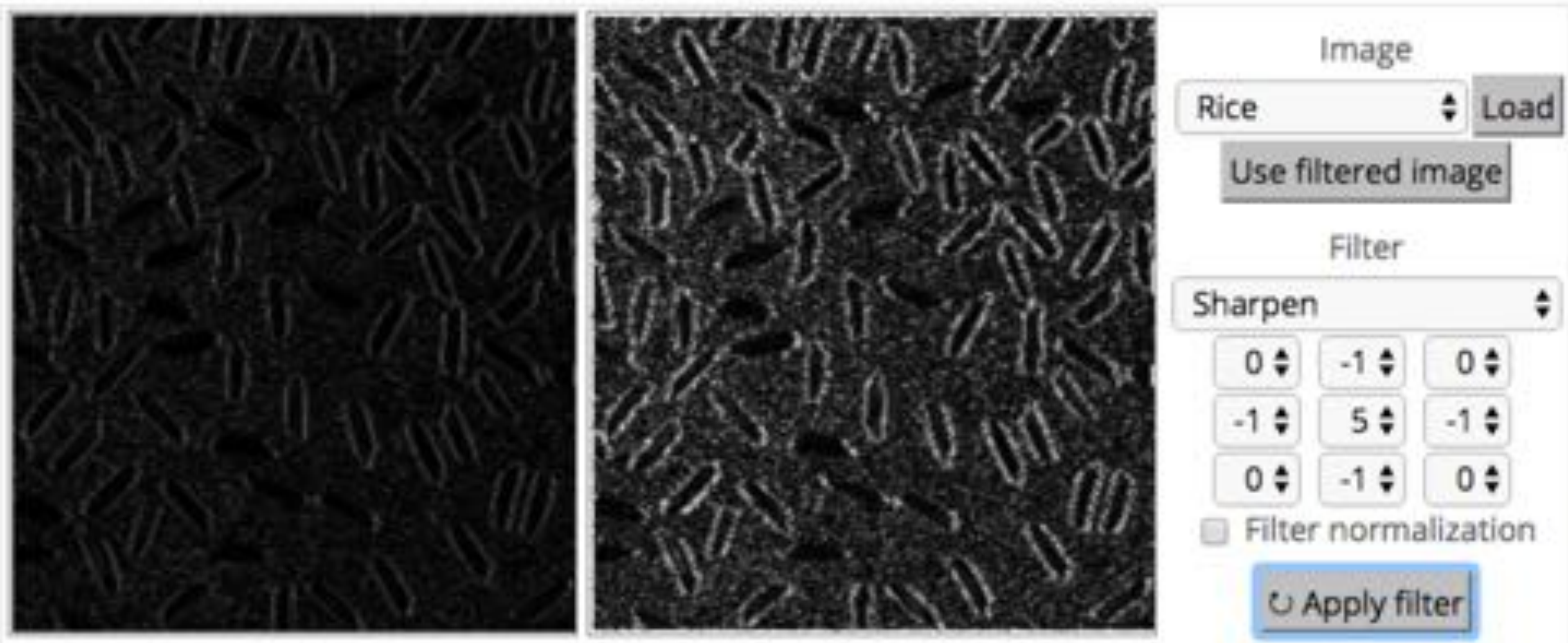

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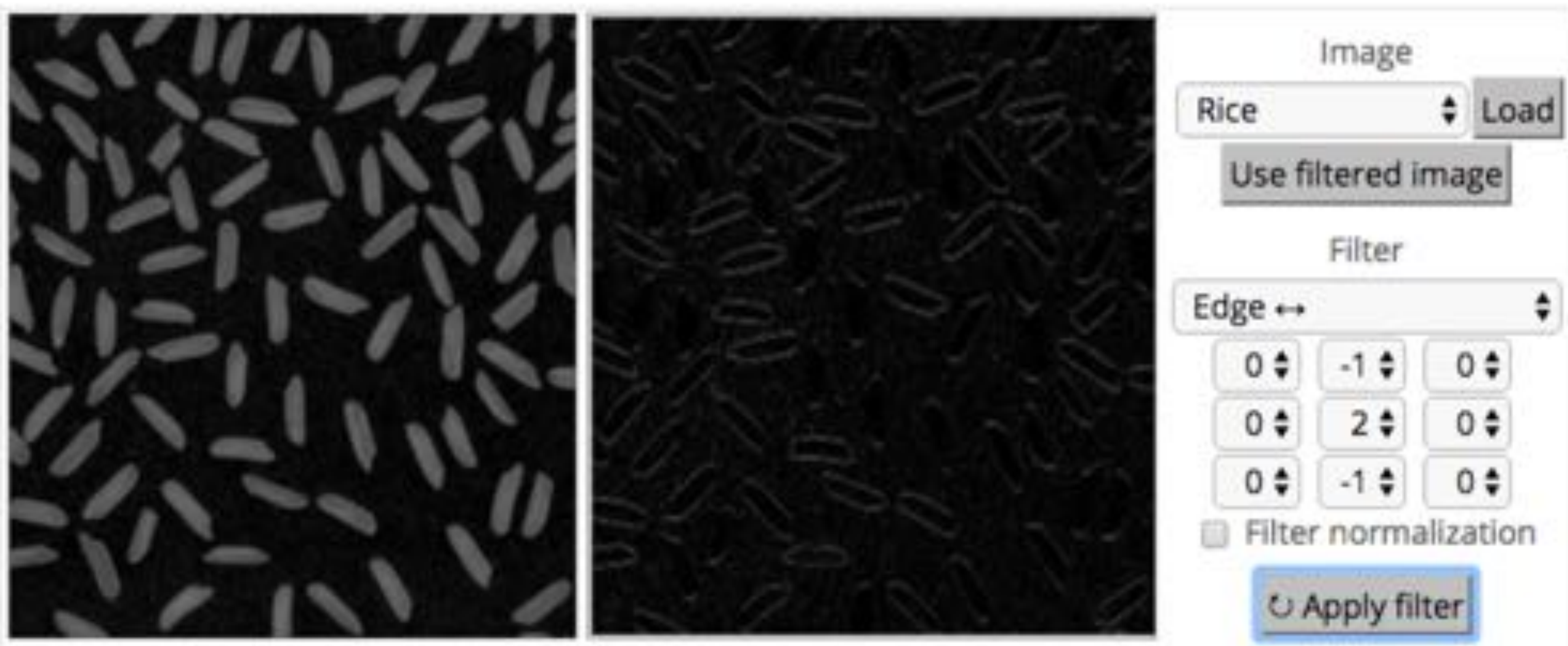

Slide from William Cohen

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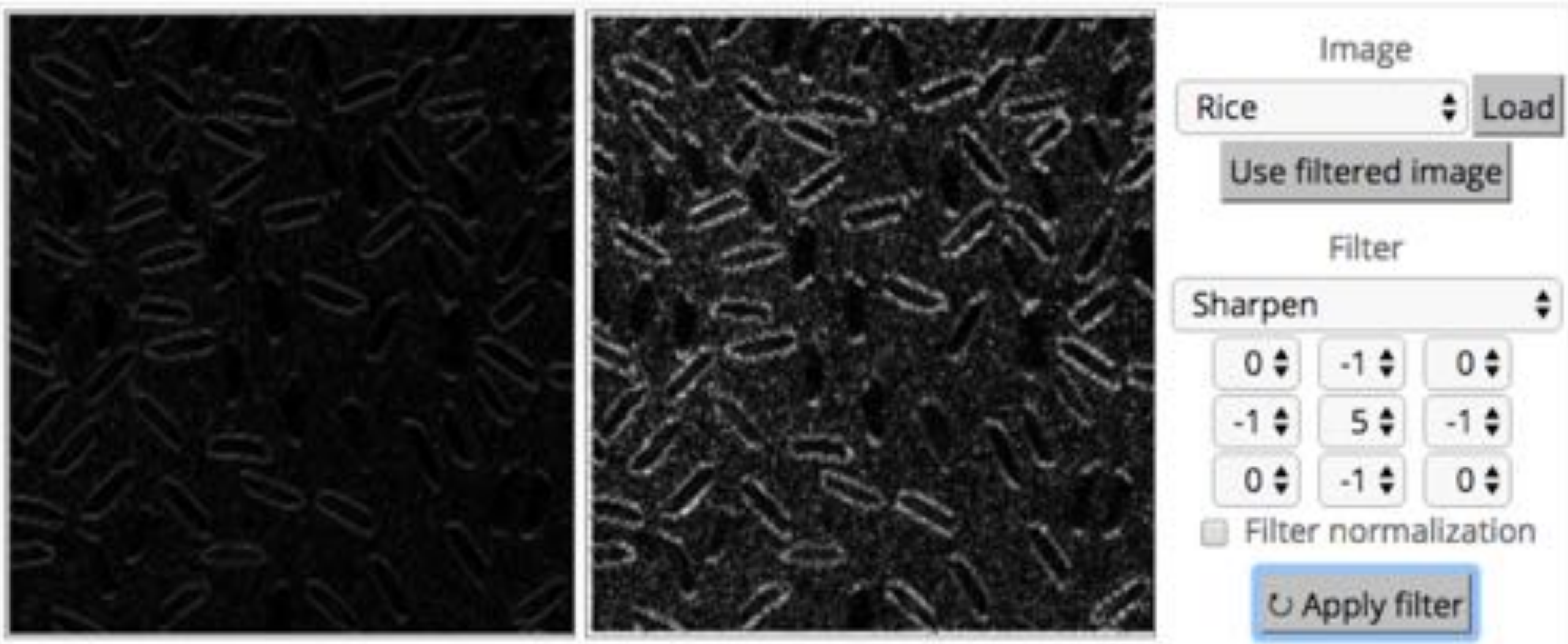

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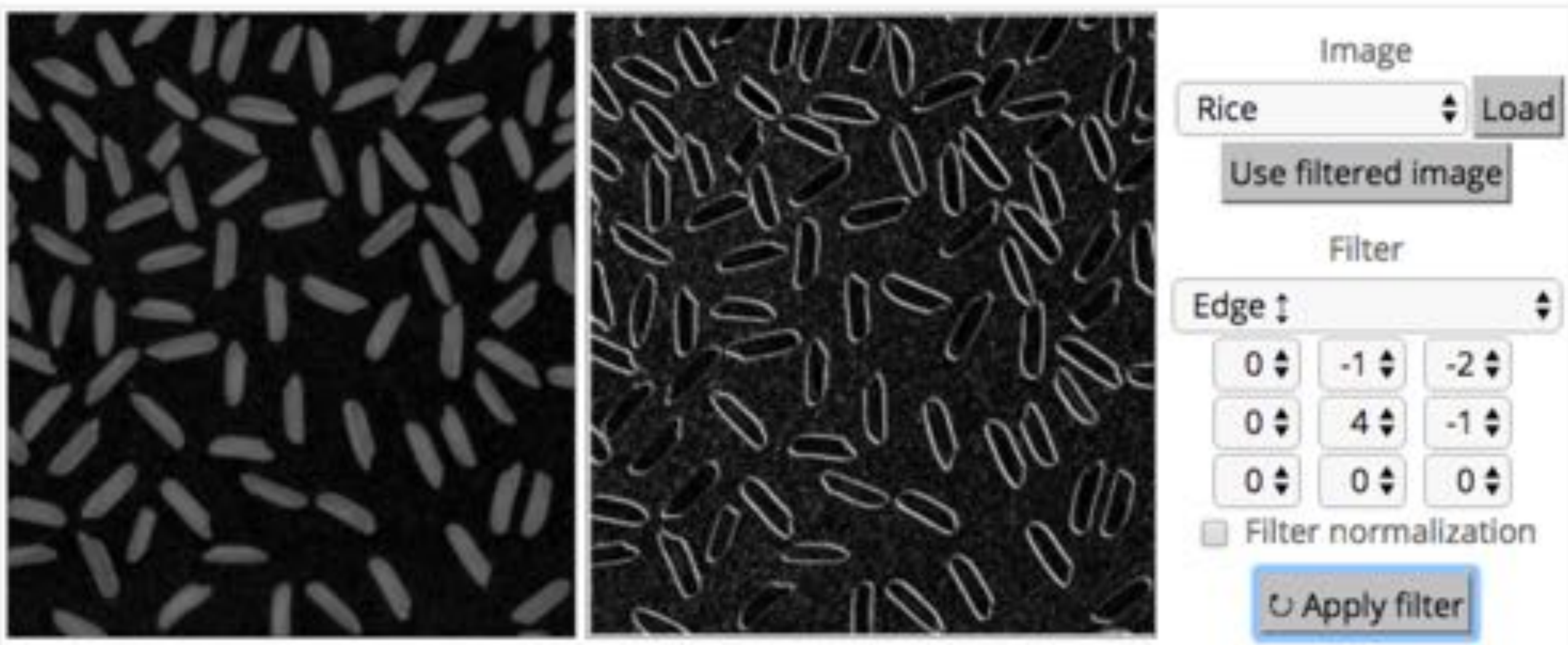

What's a convolution?

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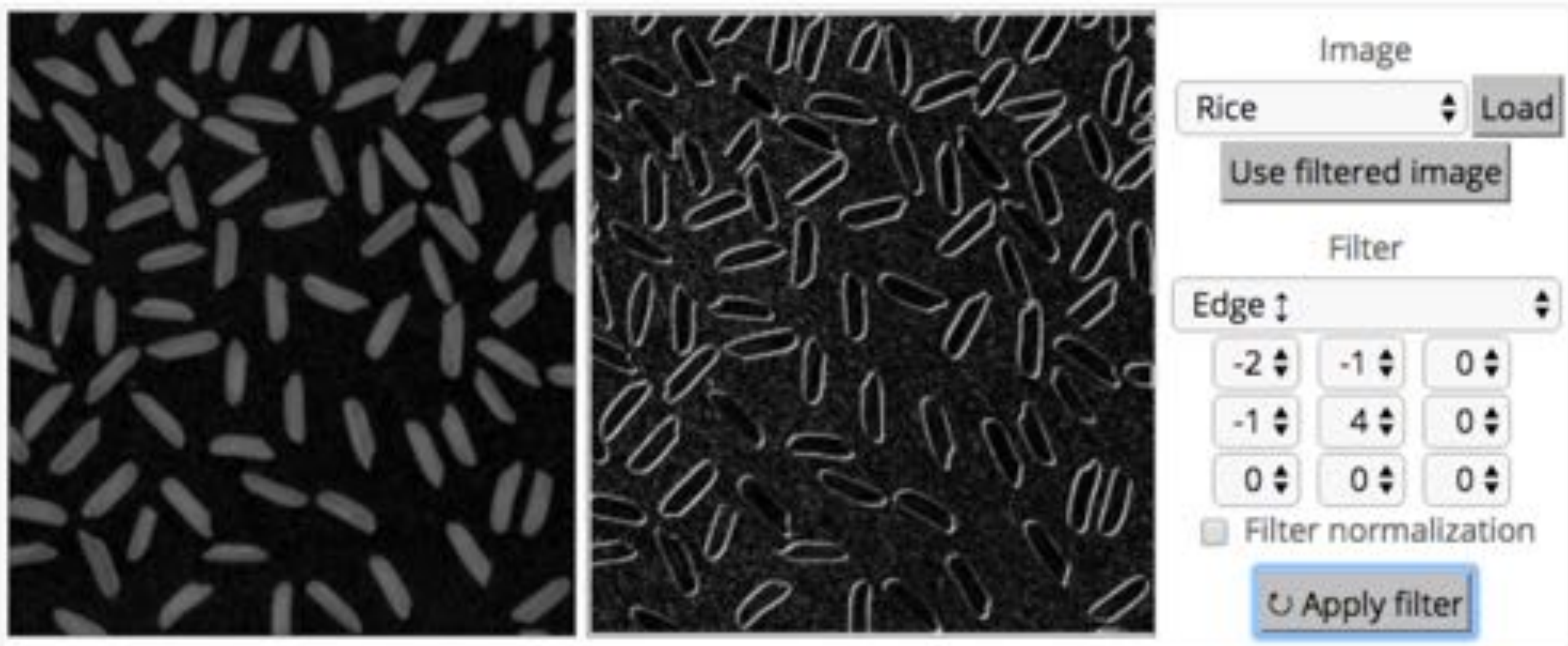


Slide from William Cohen

What's a convolution?

- Basic idea:
  - Pick a 3x3 matrix F of weights
  - Slide this over an image and compute the "inner product" (similarity) of F and the corresponding field of the image, and replace the pixel in the center of the field with the output of the inner product operation
- Key point:
  - Different convolutions extract different types of low-level "features" from an image
  - All that we need to vary to generate these different features is the weights of F

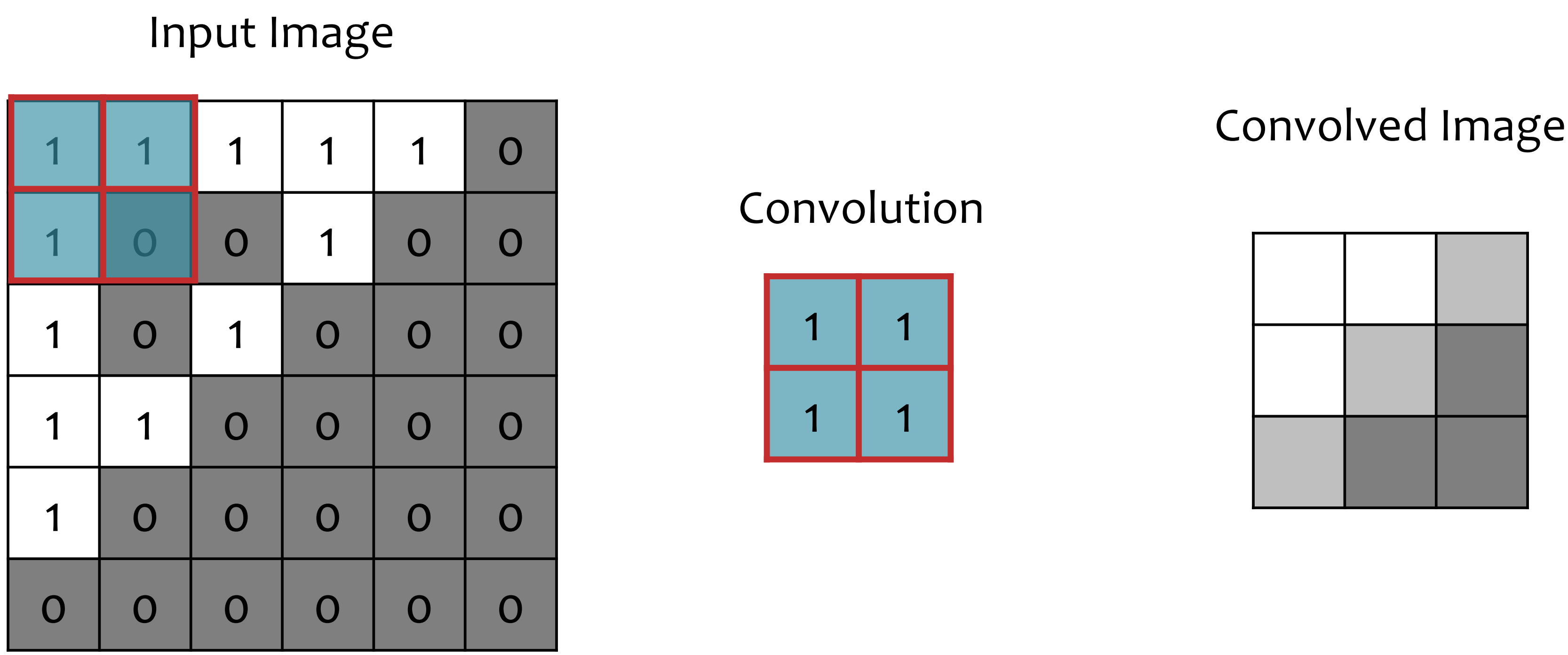
Ex: 1 input channel, 1 output channel

$$\underset{\text{Input}}{\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix}} \longrightarrow \underset{\text{Conv}}{\begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix}} \longrightarrow \underset{\text{Output}}{\begin{bmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{bmatrix}}$$

$$y_{11} = \alpha_{11} x_{11} + \alpha_{12} x_{12} + \alpha_{21} x_{21} + \alpha_{22} x_{22} + \alpha_0$$
$$y_{12} = \alpha_{11} x_{12} + \alpha_{12} x_{13} + \alpha_{21} x_{22} + \alpha_{22} x_{23} + \alpha_0$$
$$y_{21} = \alpha_{11} x_{21} + \alpha_{12} x_{22} + \alpha_{21} x_{31} + \alpha_{22} x_{32} + \alpha_0$$
$$y_{22} = \alpha_{11} x_{22} + \alpha_{12} x_{23} + \alpha_{21} x_{32} + \alpha_{22} x_{33} + \alpha_0$$

Downsampling

- Suppose we use a convolution with stride 2
- Only 9 patches visited in input, so only 9 pixels in output



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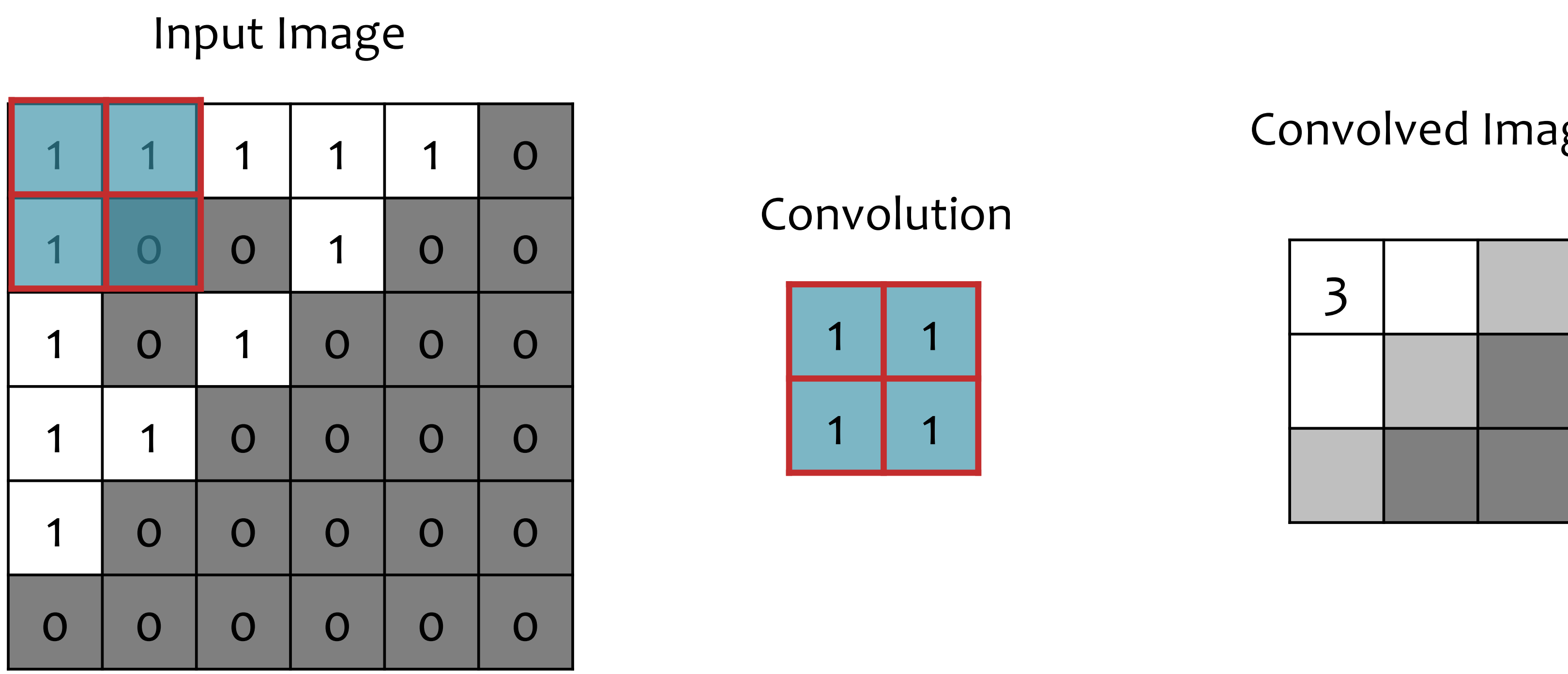

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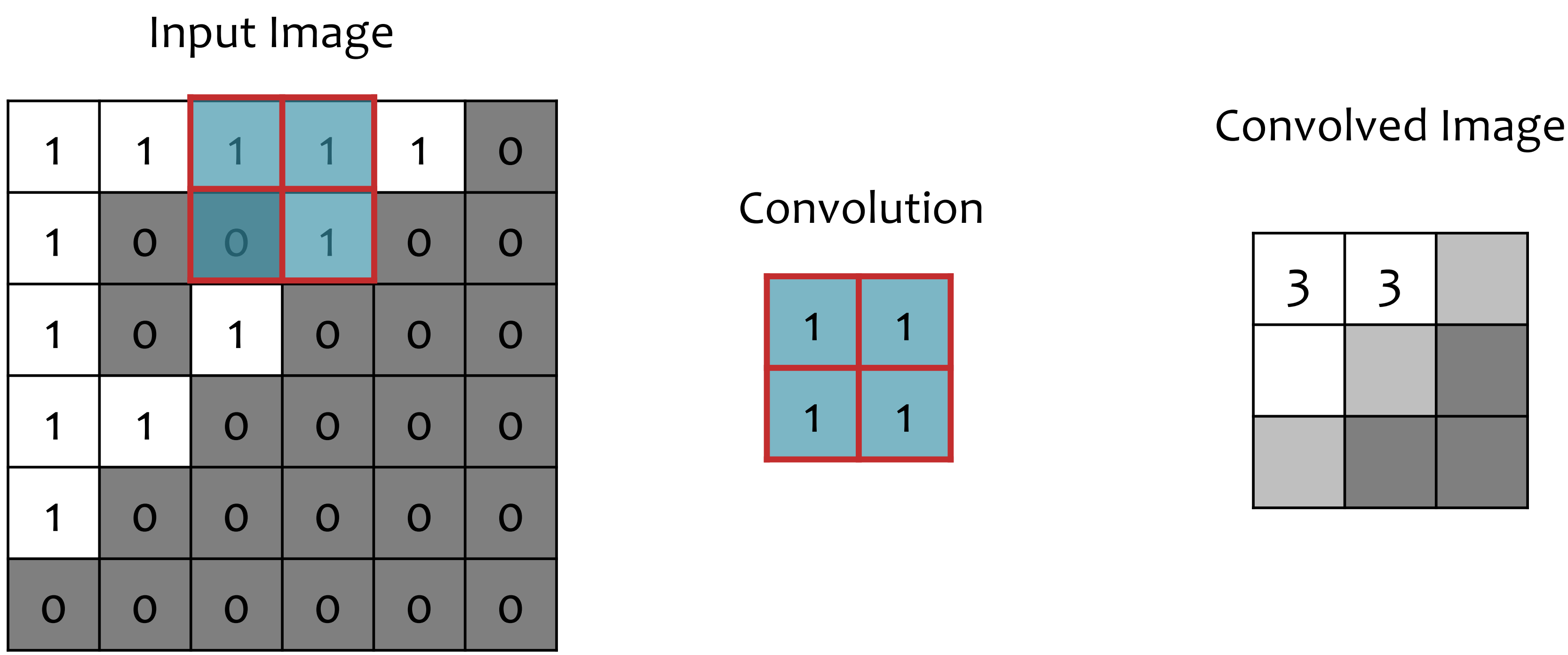

Downsampling

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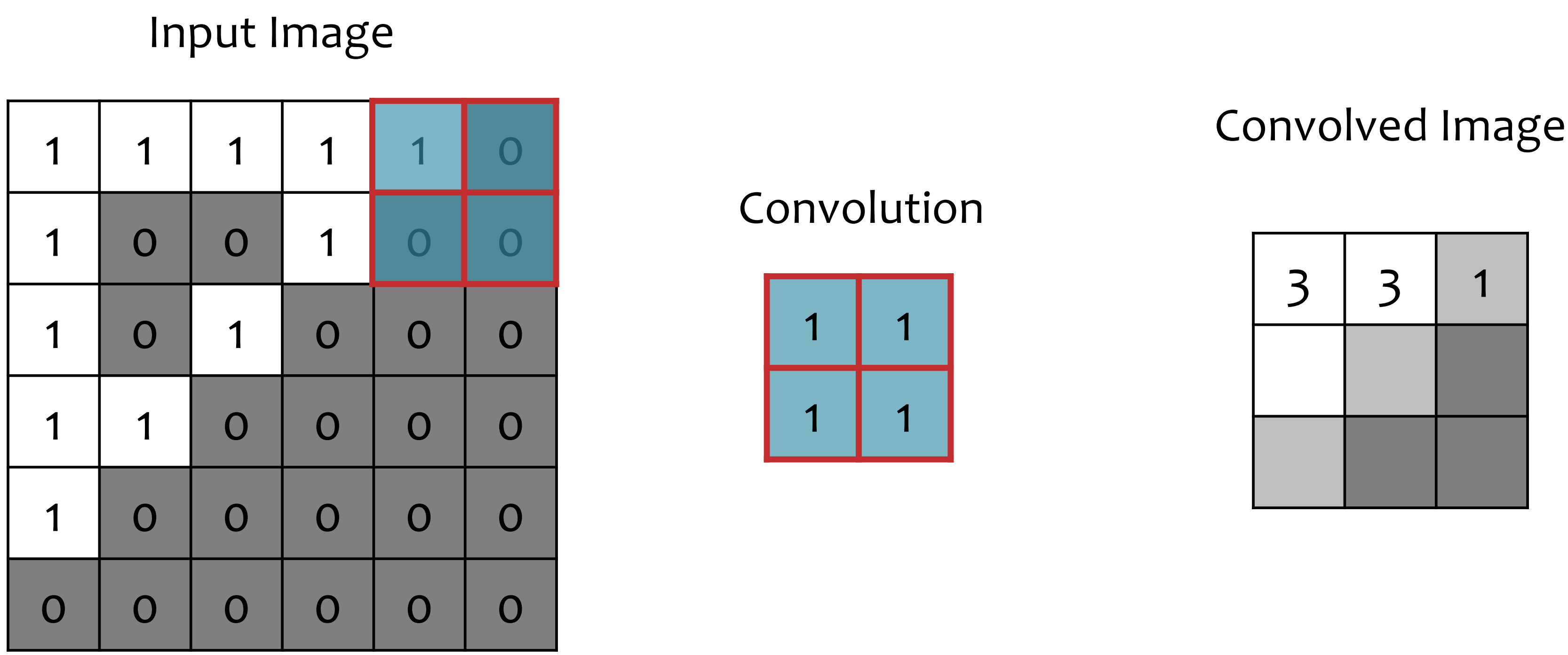

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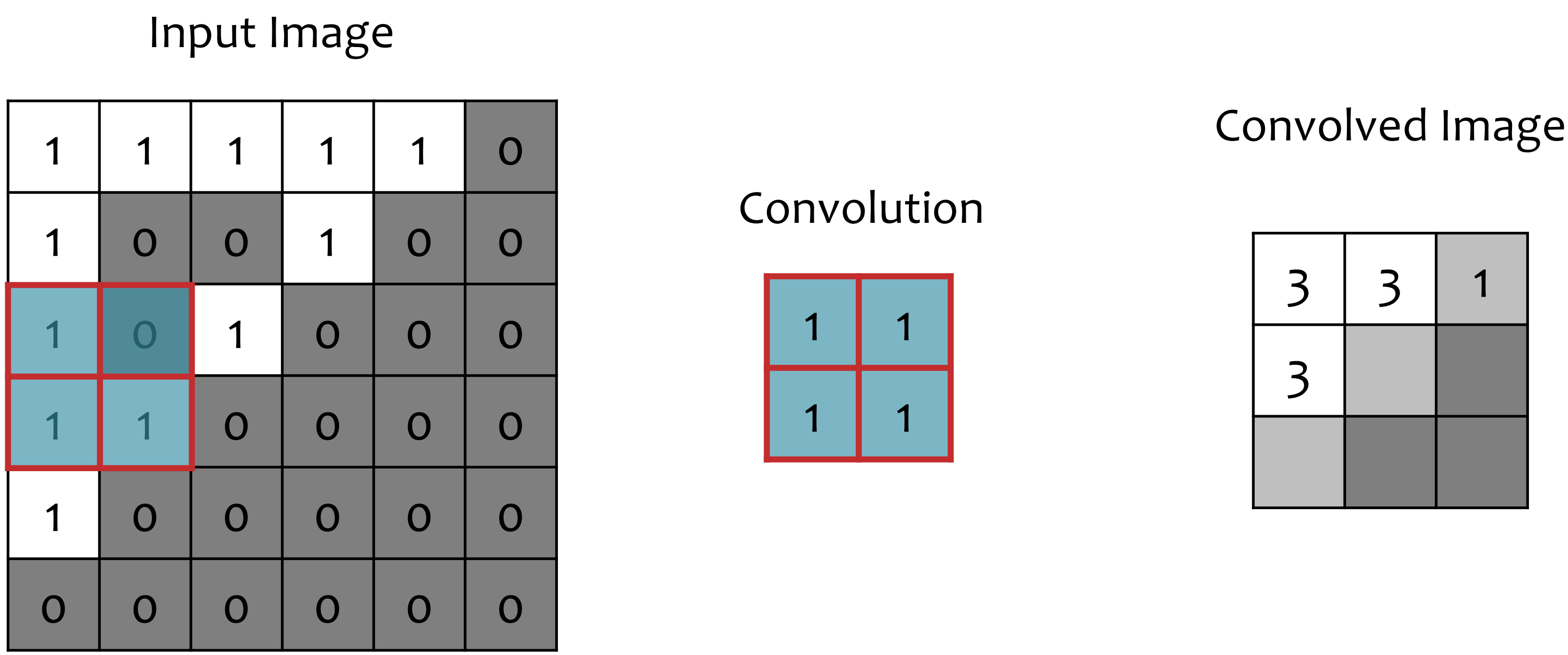

Downsampling

- Suppose we use a convolution with stride 2
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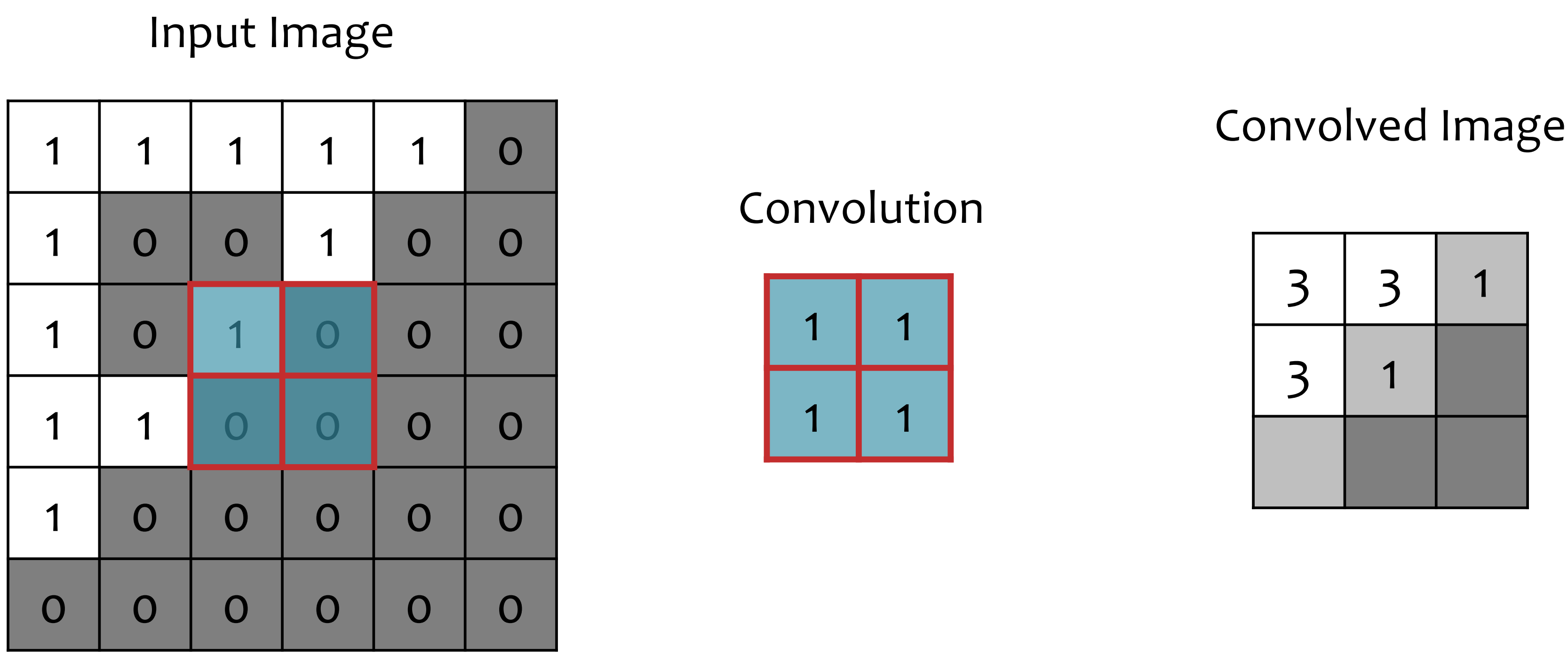
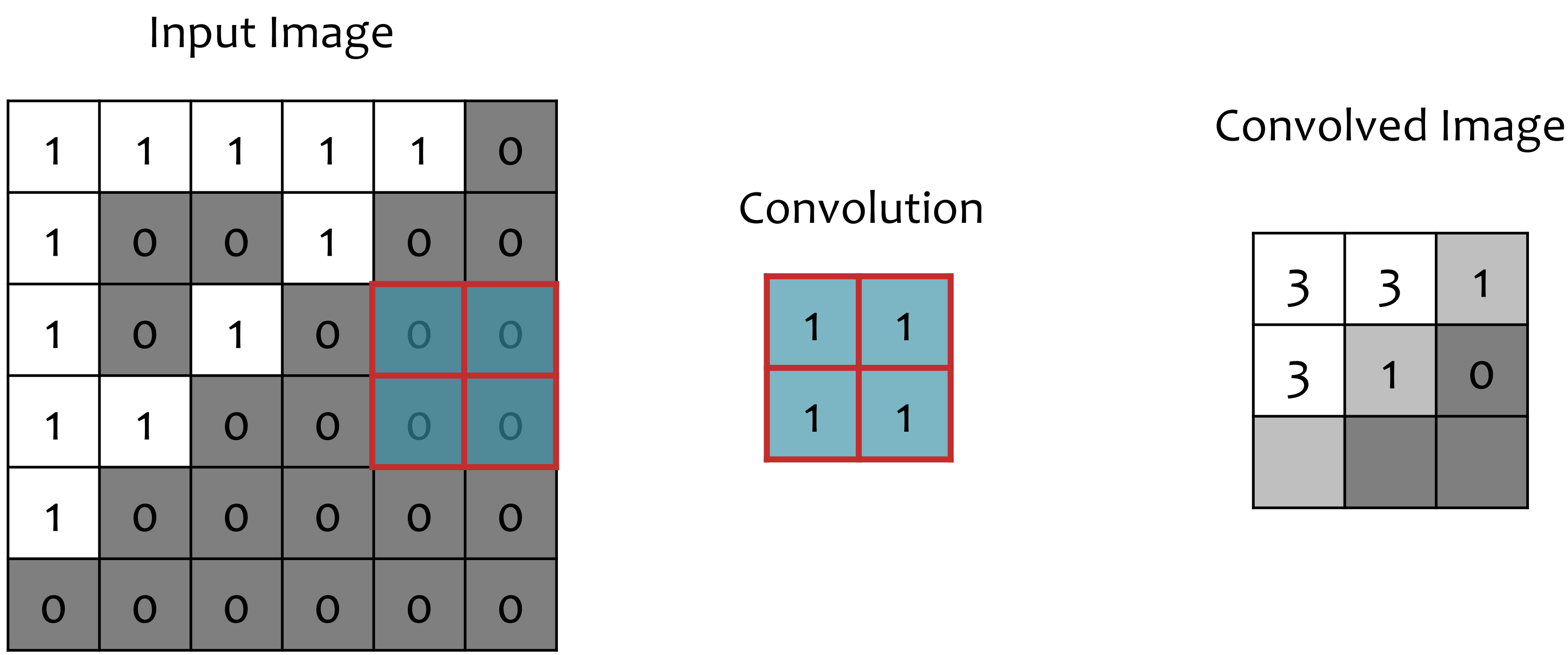


Downsampling

- Suppose we use a convolution with stride 2
- Only 9 patches visited in input, so only 9 pixels in output



Downsampling

- Suppose we use a convolution with stride 2
- Only 9 patches visited in input, so only 9 pixels in output

Input Image

1	1	1	1	1	0
1	0	0	1	0	0
1	0	1	0	0	0
1	1	0	0	0	0
1	0	0	0	0	0
0	0	0	0	0	0

Convolution

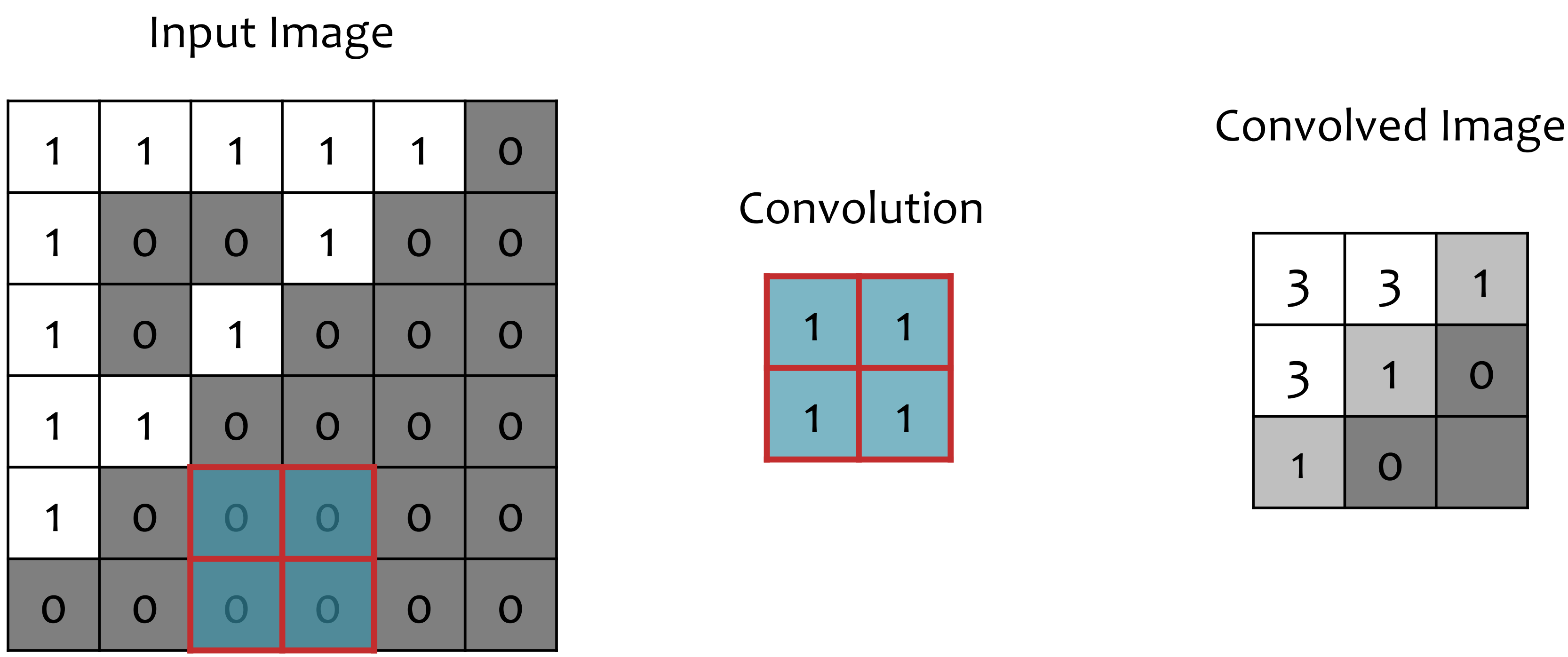
1	1
1	1

Convolved Image

3	3	1
3	1	0
1		

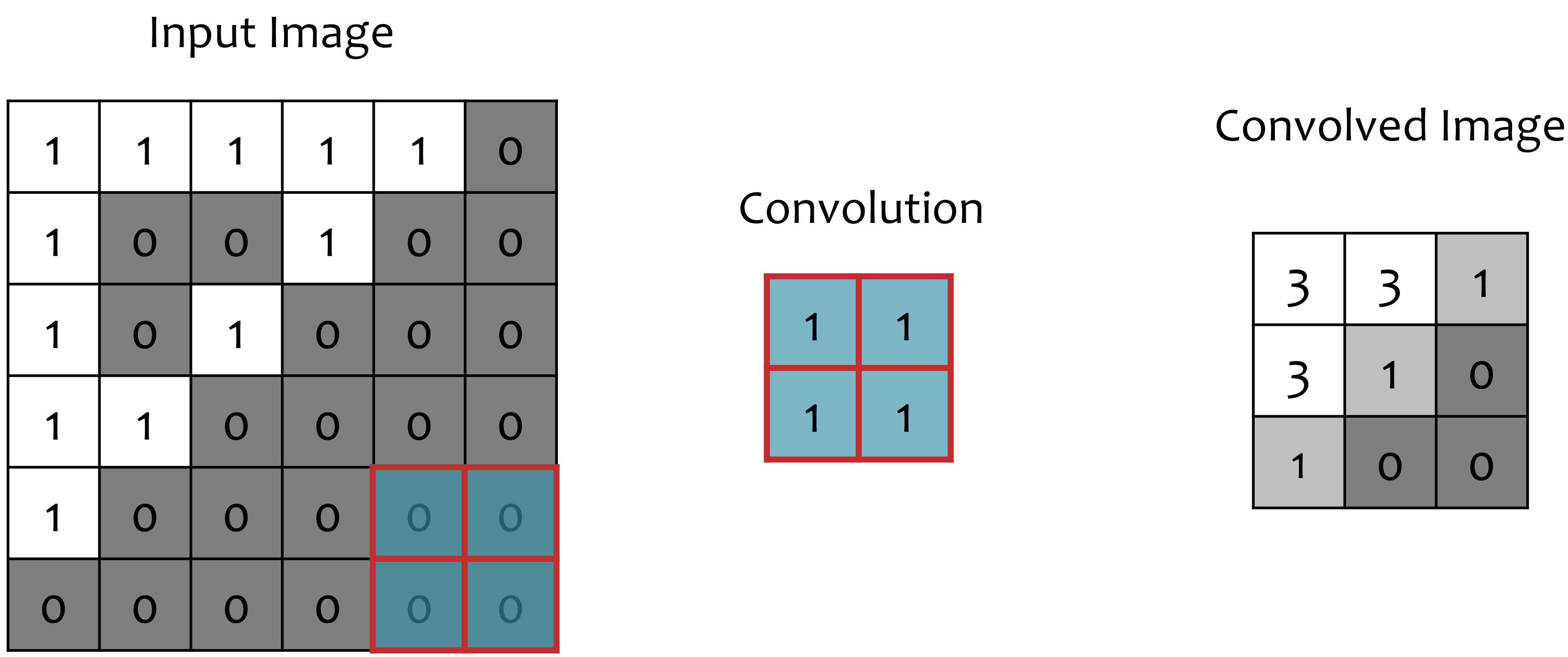
Downsampling

- Suppose we use a convolution with stride 2
- Only 9 patches visited in input, so only 9 pixels in output



Downsampling

- Suppose we use a convolution with stride 2
- Only 9 patches visited in input, so only 9 pixels in output



CONVOLUTIONAL NEURAL NETS

Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:

– Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Background

A Recipe for Machine Learning

- Convolutional Neural Networks (CNNs) provide another form of **decision function**
- Let's see what they look like…

2. Choose each of these:
   - Decision function

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

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$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Convolutional Neural Network (CNN)

- Typical layers include:
  - Convolutional layer
  - Max-pooling layer
  - Fully-connected (Linear) layer
  - ReLU layer (or some other nonlinear activation function)
  - Softmax
- These can be arranged into arbitrarily deep topologies

Architecture #1: LeNet-5

PROC. OF THE IEEE, NOVEMBER 1998 7

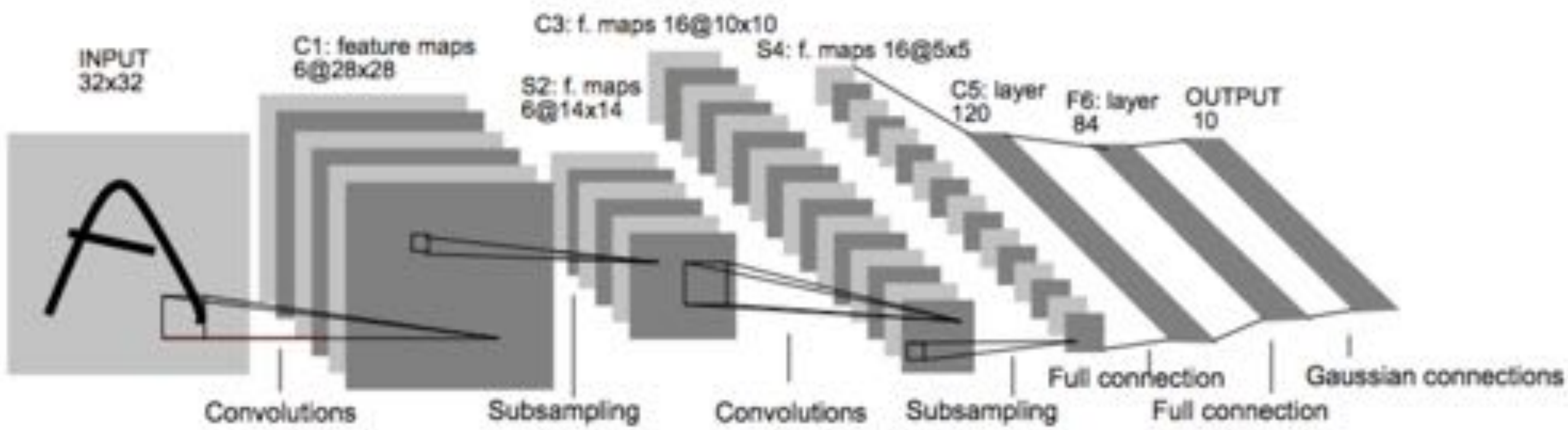


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

Convolutional Layer

CNN key idea:
Treat convolution matrix as parameters and learn them!

Input Image

0	0	0	0	0	0	0
0	1	1	1	1	1	0
0	1	0	0	1	0	0
0	1	0	1	0	0	0
0	1	1	0	0	0	0
0	1	0	0	0	0	0
0	0	0	0	0	0	0

Learned Convolution

θ_{11}	θ_{12}	θ_{13}
θ_{21}	θ_{22}	θ_{23}
θ_{31}	θ_{32}	θ_{33}

Convolved Image

.4	.5	.5	.5	.4
.4	.2	.3	.6	.3
.5	.4	.4	.2	.1
.5	.6	.2	.1	0
.4	.3	.1	0	0

Downsampling by Averaging

- Downsampling by averaging **used to be** a common approach
- This is a special case of convolution where the weights are fixed to a uniform distribution
- The example below uses a stride of 2

Input Image

1	1	1	1	1	0
1	0	0	1	0	0
1	0	1	0	0	0
1	1	0	0	0	0
1	0	0	0	0	0
0	0	0	0	0	0

Convolution

1/4	1/4
1/4	1/4

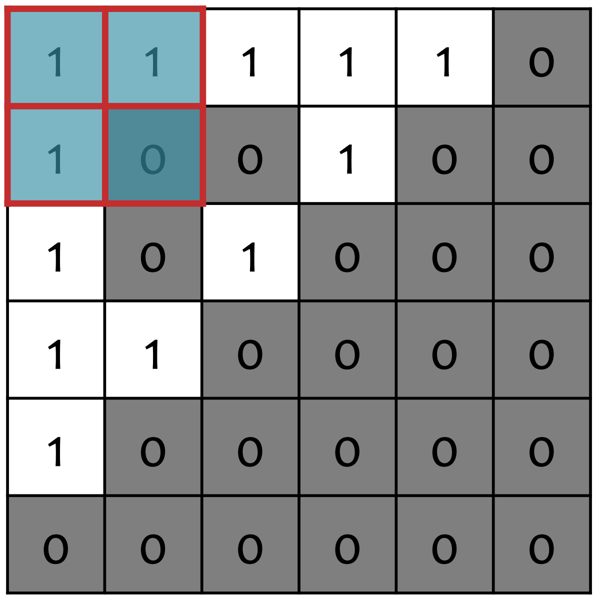
Convolved Image

3/4	3/4	1/4
3/4	1/4	0
1/4	0	0

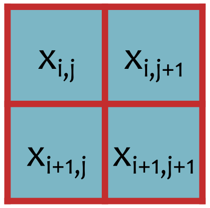
Max-Pooling

- Max-pooling is another (common) form of downsampling
- Instead of averaging, we take the max value within the same range as the equivalently-sized convolution
- The example below uses a stride of 2

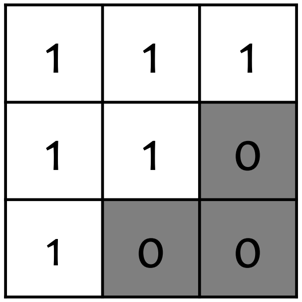
Input Image



Max-pooling



Max-Pooled Image



$$y_{ij} = \max(x_{ij}, x_{i,j+1}, x_{i+1,j}, x_{i+1,j+1})$$

TRAINING CNNS

Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:

– Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:
(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Background

A Recipe for Machine Learning

1. Given training data:

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– Decision function

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

- Q: Now that we have the CNN as a decision function, how do we compute the gradient?
- A: Backpropagation of course!

opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

SGD for CNNs

SGD for CNNs

Ex: Architecture: Given $\vec{x}, y^*$

$J = \ell(y, y^*)$

$y = \text{softmax}(z^{(5)})$

$z^{(5)} = \text{linear}(z^{(4)}, W)$

$z^{(4)} = \text{relu}(z^{(3)})$

$z^{(3)} = \text{conv}(z^{(2)}, \beta)$

$z^{(2)} = \text{max-pool}(z^{(1)})$

$z^{(1)} = \text{conv}(\vec{x}, \alpha)$

Parameters $\vec{\Theta} = [\alpha, \beta, W]$

SGD:

① Init $\vec{\Theta}$

② While not converged:

Sample $i \in \{1, \dots, N\}$

Forward: $y = h_{\Theta}(\vec{x}^{(i)})$, $J_i(\Theta) = \ell(y, y^*)$

Backward: $\nabla_{\vec{\Theta}} J_i(\Theta) = \dots$

Update: $\vec{\Theta} \leftarrow \vec{\Theta} - \lambda \nabla_{\vec{\Theta}} J_i(\Theta)$

LAYERS OF A CNN

Common CNN Layers

Whiteboard

- ReLU Layer
- Background: Subgradient
- Fully-connected Layer (w/tensor input)
- Softmax Layer
- Convolutional Layer
- Max-Pooling Layer

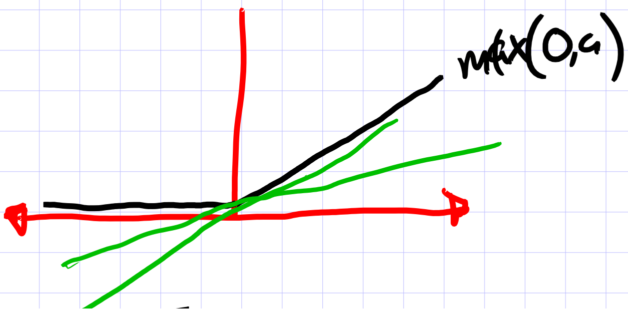
ReLU Layer

ReLU Layer Input: $\vec{x} \in \mathbb{R}^K$ Output: $\vec{y} \in \mathbb{R}^K$

Forward:

$\vec{y} = \sigma(\vec{x})$ ← element-wise

$\sigma(a) = \max(0, a)$



Backward:

$$\frac{dJ}{dx_i} = \frac{dJ}{dy_i} \frac{dy_i}{dx_i}$$

subderivative

where $\frac{dy_i}{dx_i} = \begin{cases} 1 & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$

Softmax Layer

$\boxed{\text{Softmax Layer}}$

Input: $\vec{x} \in \mathbb{R}^K$ Output: $\vec{y} \in \mathbb{R}^K$

Forward:

$$y_i = \frac{\exp(x_i)}{\sum_{k=1}^{K} \exp(x_k)}$$

Backward:

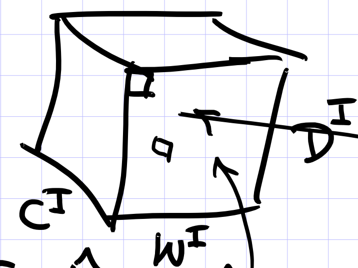
$$\frac{dJ}{dx_j} = \sum_{i=1}^{K} \frac{dJ}{dy_i} \frac{dy_i}{dx_j}$$

where $\frac{dy_i}{dx_j} = \begin{cases} y_i(1-y_i) & \text{if } i=j \\ -y_i y_j & \text{otherwise} \end{cases}$

Fully-Connected Layer

Fully Connected Layer (w/ tensor input)

- Suppose input is a 3D Tensor: $X =$



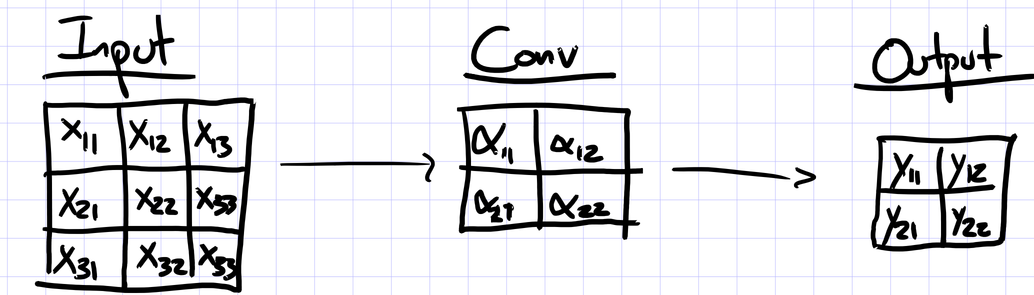
- stretch out into a long vector: $\hat{X} = [\hat{x}_1, \ldots, \hat{x}_{(C \times H \times W)}]$
- then standard linear layer:

$$y = \alpha^T \hat{x} + \alpha_0 \quad \text{where } \alpha \in \mathbb{R}^{A \times B}$$

$$|\hat{x}| = A, \; |y| = B$$

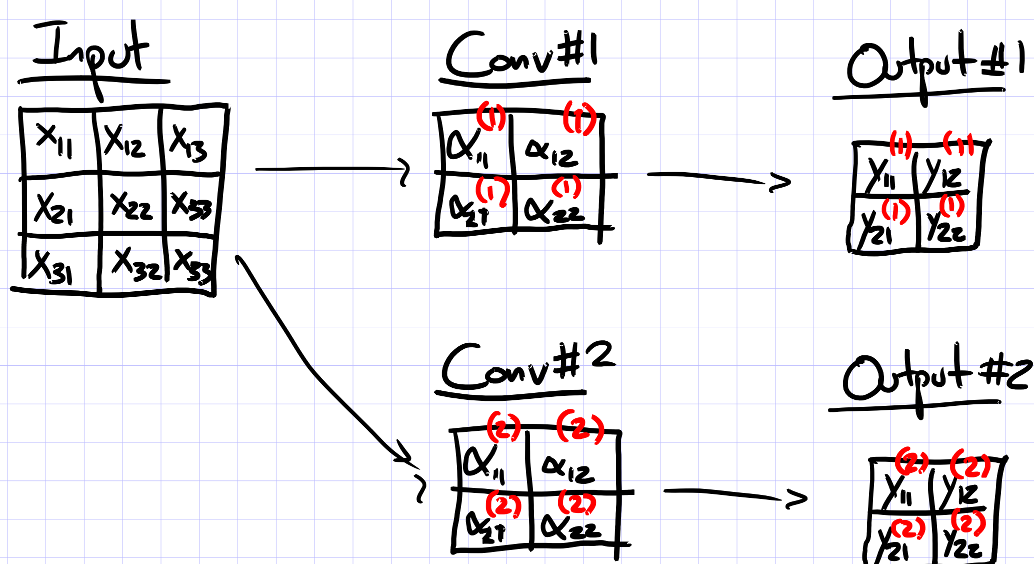
Convolutional Layer

Ex: 1 input channel, 1 output channel



$$y_{11} = \alpha_{11} x_{11} + \alpha_{12} x_{12} + \alpha_{21} x_{21} + \alpha_{22} x_{22} + \alpha_0$$
$$y_{12} = \alpha_{11} x_{12} + \alpha_{12} x_{13} + \alpha_{21} x_{22} + \alpha_{22} x_{23} + \alpha_0$$
$$y_{21} = \alpha_{11} x_{21} + \alpha_{12} x_{22} + \alpha_{21} x_{31} + \alpha_{22} x_{32} + \alpha_0$$
$$y_{22} = \alpha_{11} x_{22} + \alpha_{12} x_{23} + \alpha_{21} x_{32} + \alpha_{22} x_{33} + \alpha_0$$

Ex: 1 input channel, 2 output channels



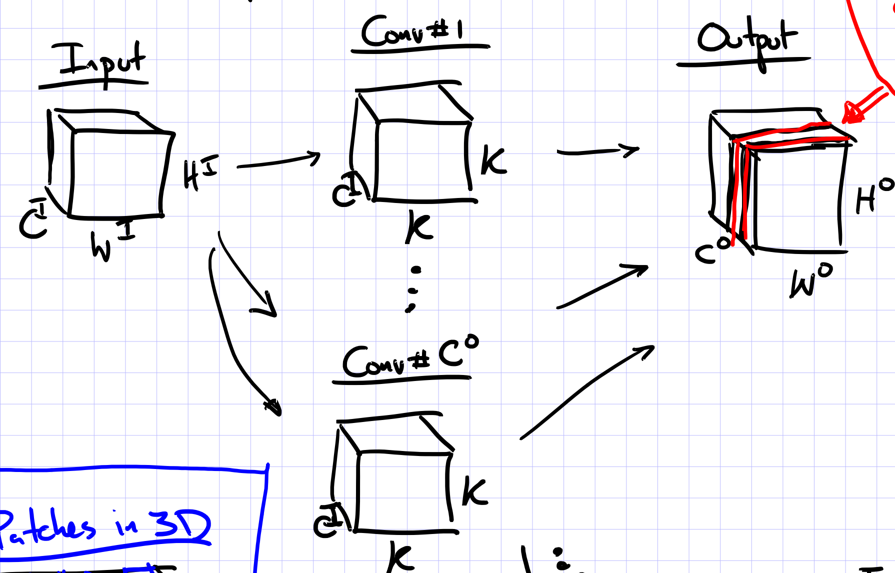
$$y_{11}^{(1)} = \alpha_{11}^{(1)} x_{11} + \alpha_{12}^{(1)} x_{12} + \alpha_{21}^{(1)} x_{21} + \alpha_{22}^{(1)} x_{22} + \alpha_0^{(1)}$$
$$y_{12}^{(1)} = \cdots$$
$$y_{21}^{(1)} = \cdots$$
$$y_{22}^{(1)} = \alpha_{11}^{(1)} x_{22} + \alpha_{12}^{(1)} x_{23} + \alpha_{21}^{(1)} x_{32} + \alpha_{22}^{(1)} x_{33} + \alpha_0^{(1)}$$

$$y_{11}^{(2)} = \alpha_{11}^{(2)} x_{11} + \alpha_{12}^{(2)} x_{12} + \alpha_{21}^{(2)} x_{21} + \alpha_{22}^{(2)} x_{22} + \alpha_0^{(2)}$$
$$y_{12}^{(2)} = \cdots$$
$$y_{21}^{(2)} = \cdots$$
$$y_{22}^{(2)} = \alpha_{11}^{(2)} x_{22} + \alpha_{12}^{(2)} x_{23} + \alpha_{21}^{(2)} x_{32} + \alpha_{22}^{(2)} x_{33} + \alpha_0^{(2)}$$

Convolutional Layer

Ex: C^I input channels, C^I output channels

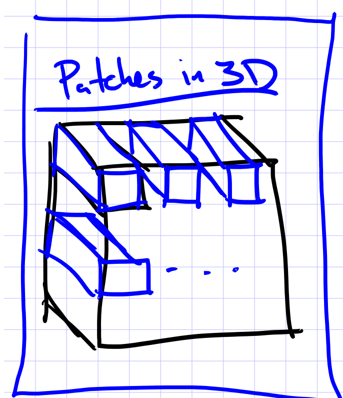
jth slice is output from jth convolution matrix



$$H^O = \lfloor (H^I + 2p - K)/s + 1 \rfloor$$

$$W^O = \lfloor (W^I + 2p - K)/s + 1 \rfloor$$

where p = # pixels of padding on input
K = size of conv. matrix
s = stride length



Forward:

$$y_{ij}^{(k)} = \alpha_0^{(k)} + \sum_{c=1}^{C^I} \sum_{q=1}^{K} \sum_{r=1}^{K} \alpha_{qr}^{(k)} x_{mn}^{(c)} \quad \text{where} \quad m = s(i-1)+q, \; n = s(j-1)+r$$

Backward:

$$\frac{dJ}{d\alpha_0^{(k)}} = \sum_i \sum_j \frac{dJ}{dy_{ij}^{(k)}} \frac{dy_{ij}^{(k)}}{d\alpha_0^{(k)}}$$

$$\frac{dJ}{d\alpha_{qr}^{(k)}} = \sum_i \sum_j \frac{dJ}{dy_{ij}^{(k)}} \frac{dy_{ij}^{(k)}}{d\alpha_{qr}^{(k)}}$$

$$\frac{dJ}{dx_{mn}^{(c)}} = \sum_i \sum_j \sum_k \frac{dJ}{dy_{ij}^{(k)}} \frac{dy_{ij}^{(k)}}{dx_{mn}^{(c)}}$$

just some calculus

Max-Pooling Layer

Ex: 1 input channel, 1 output channel, stride of 1

Input

x_{11}	x_{12}	x_{13}
x_{21}	x_{22}	x_{23}
x_{31}	x_{32}	x_{33}

$\longrightarrow$

Pool Size

$\longrightarrow$

Output

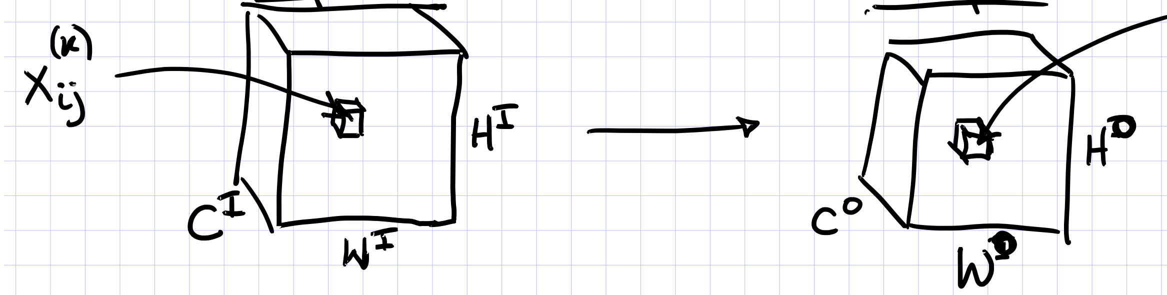
y_{11}	y_{12}
y_{21}	y_{22}

$$y_{11} = \max(x_{11}, x_{12}, x_{21}, x_{22})$$
$$y_{12} = \max(x_{12}, x_{13}, x_{22}, x_{23})$$
$$y_{21} = \max(x_{21}, x_{22}, x_{31}, x_{32})$$
$$y_{22} = \max(x_{22}, x_{23}, x_{32}, x_{33})$$

Max-Pooling Layer

Max-Pooling Layer

Input: Output:



$C^O = C^I$

$H^O = \dots$
$W^O = \dots$ } same as conv. layer

Same hyperparams too.

Forward:

$$y_{ij}^{(k)} = \max_{\substack{q\in\{1,\dots,K\}\\ r\in\{1,\dots,K\}}} x_{mn}^{(k)} \quad \text{where} \quad \begin{array}{l} m = s(i-1)+q \\ n = s(j-1)+r \end{array}$$

Backward:

$$\frac{dJ}{dx_{mn}^{(k)}} = \sum_i \sum_j \frac{dJ}{dy_{ij}^{(k)}} \frac{dy_{ij}^{(k)}}{dx_{mn}^{(k)}}$$

Subderivatives

+ Max() is not differentiable, but subdifferentiable.
+ There are a set of derivatives and we can just choose one for SGD.

$y = \max(a,b)$

$$\Rightarrow \frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da} \quad \text{where} \quad \frac{dy}{da} = \begin{cases} 1 & \text{if } a > b \\ 0 & \text{otherwise} \end{cases}$$

Convolutional Neural Network (CNN)

- Typical layers include:
  - Convolutional layer
  - Max-pooling layer
  - Fully-connected (Linear) layer
  - ReLU layer (or some other nonlinear activation function)
  - Softmax
- These can be arranged into arbitrarily deep topologies

Architecture #1: LeNet-5

PROC. OF THE IEEE, NOVEMBER 1998 7

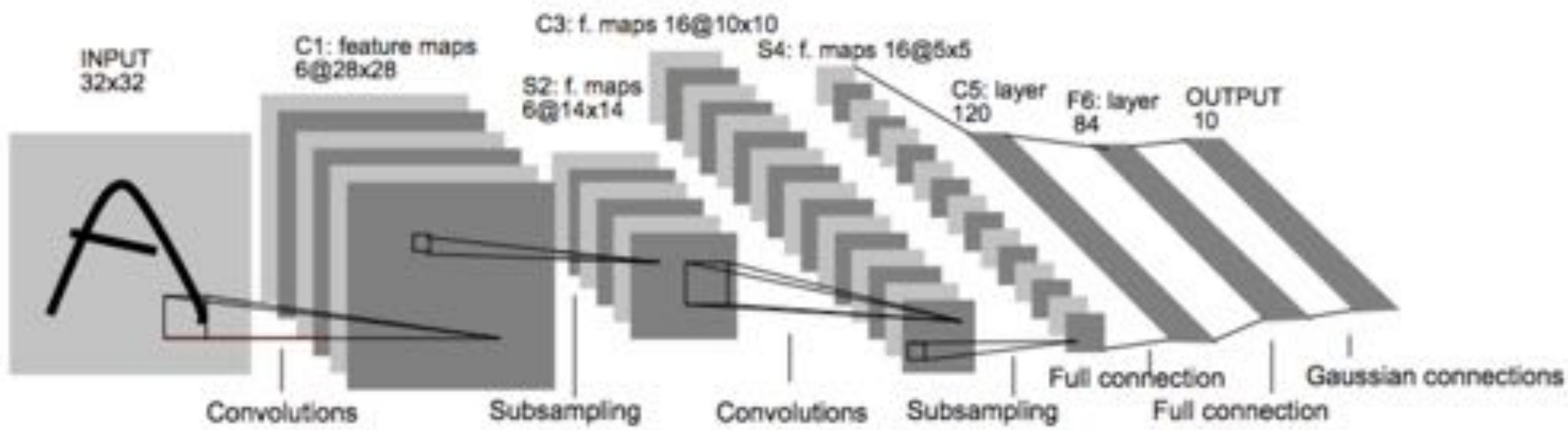


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

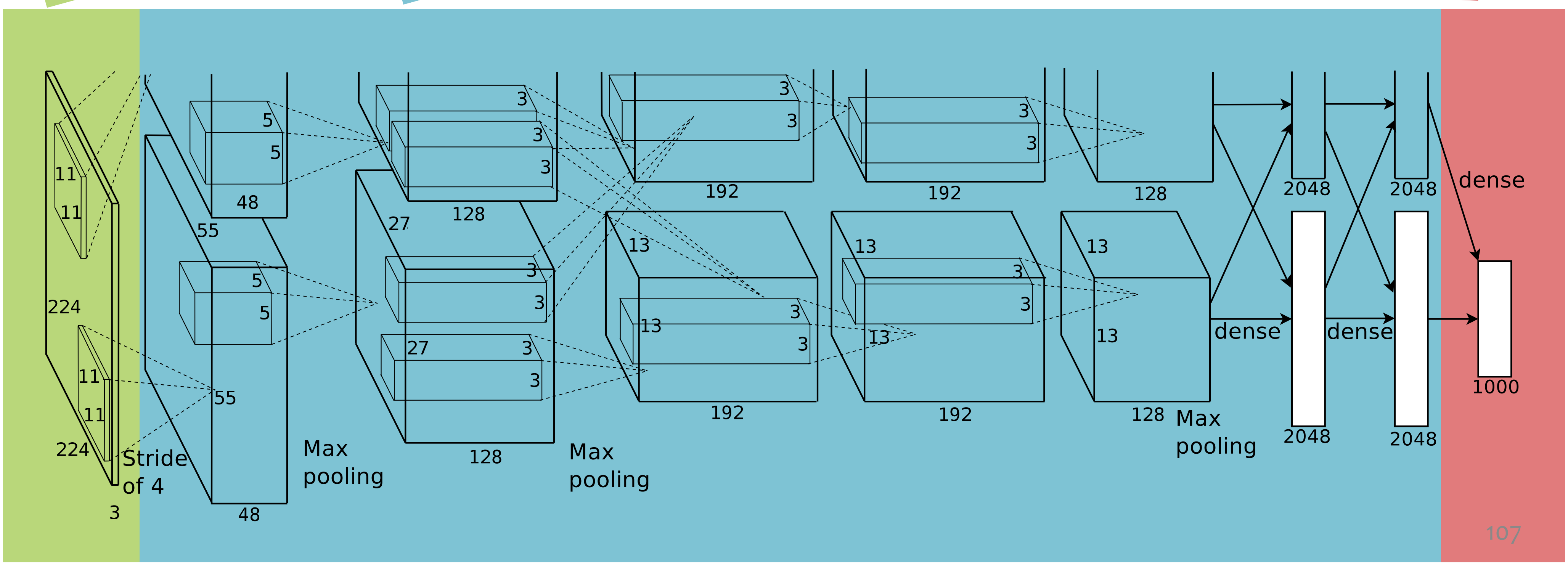
Architecture #2: AlexNet

CNN for Image Classification
(Krizhevsky, Sutskever & Hinton, 2012)
15.3% error on ImageNet LSVRC-2012 contest

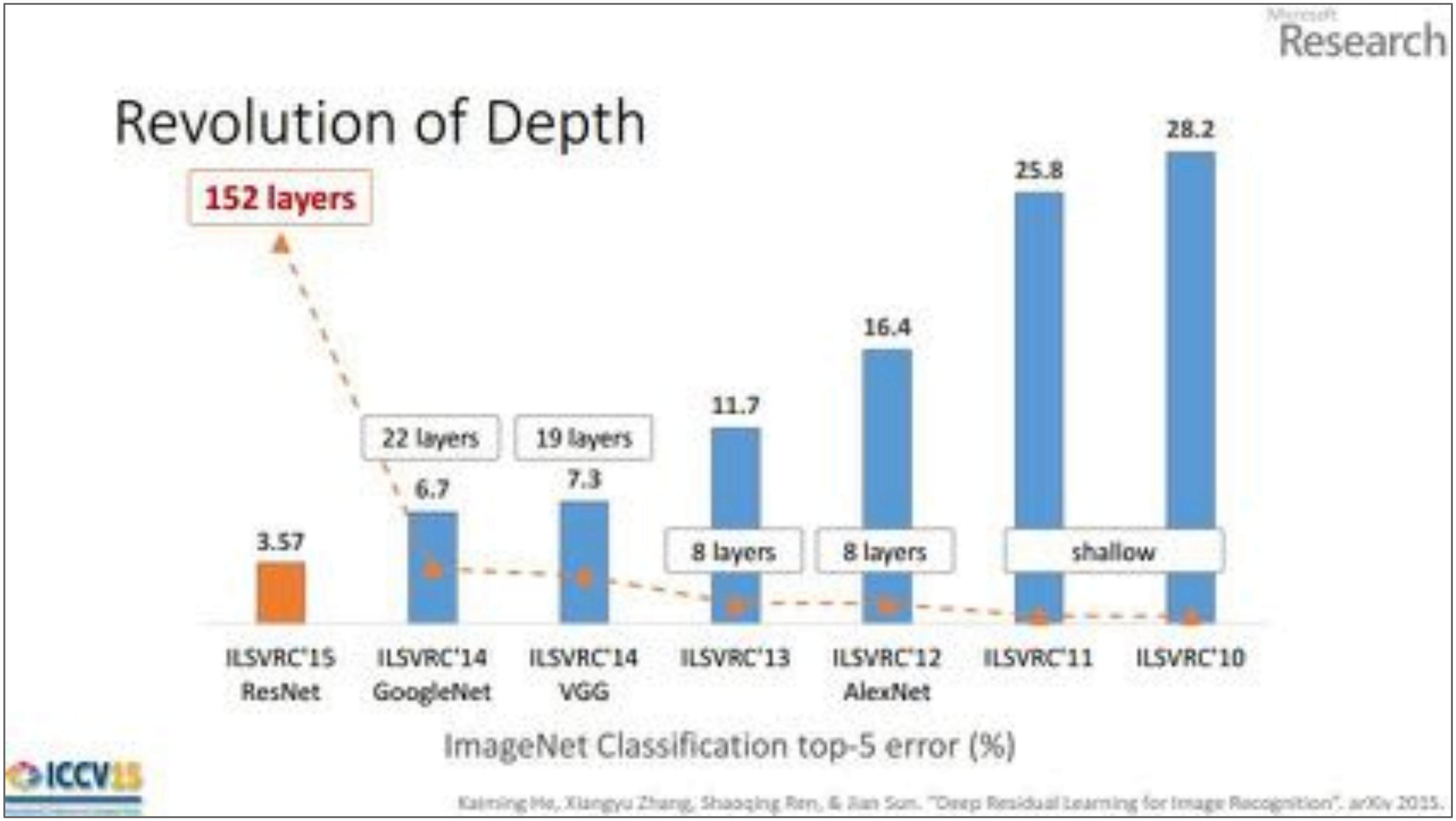
Input image (pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

1000-way softmax



CNNs for Image Recognition

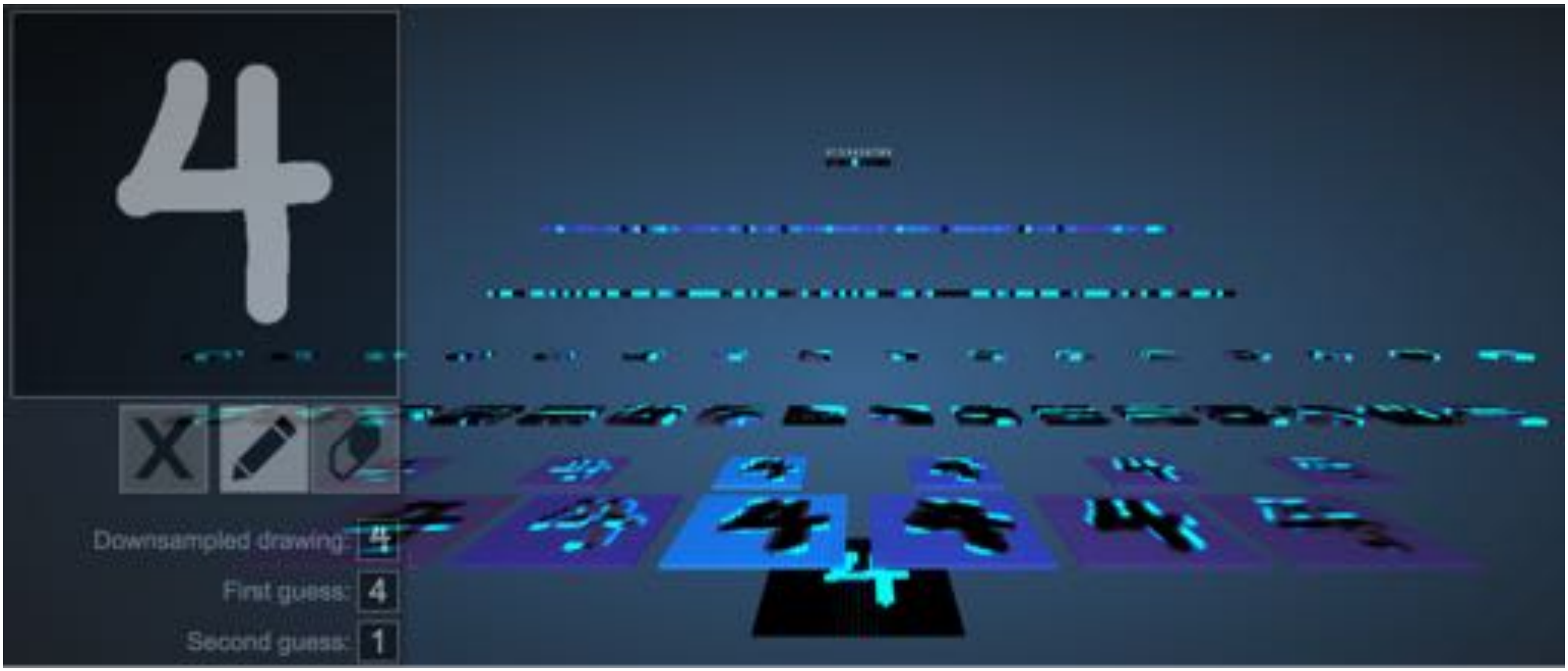


Slide from Kaiming He

CNN VISUALIZATIONS

3D Visualization of CNN

http://scs.ryerson.ca/~aharley/vis/conv/



Convolution of a Color Image

- Color images consist of 3 floats per pixel for RGB (red, green blue) color values
- Convolution must also be 3-dimensional

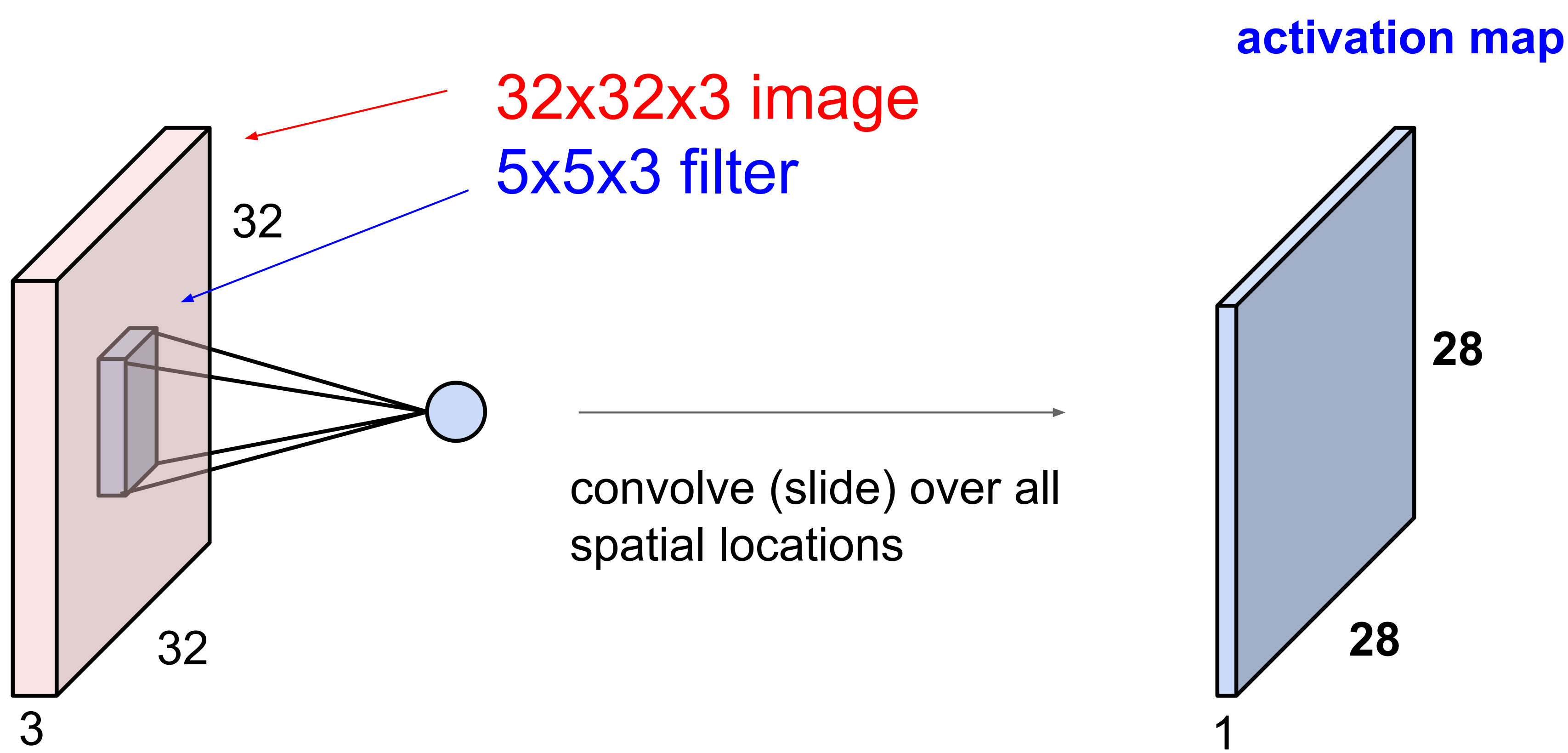


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

Animation of 3D Convolution

http://cs231n.github.io/convolutional-networks/

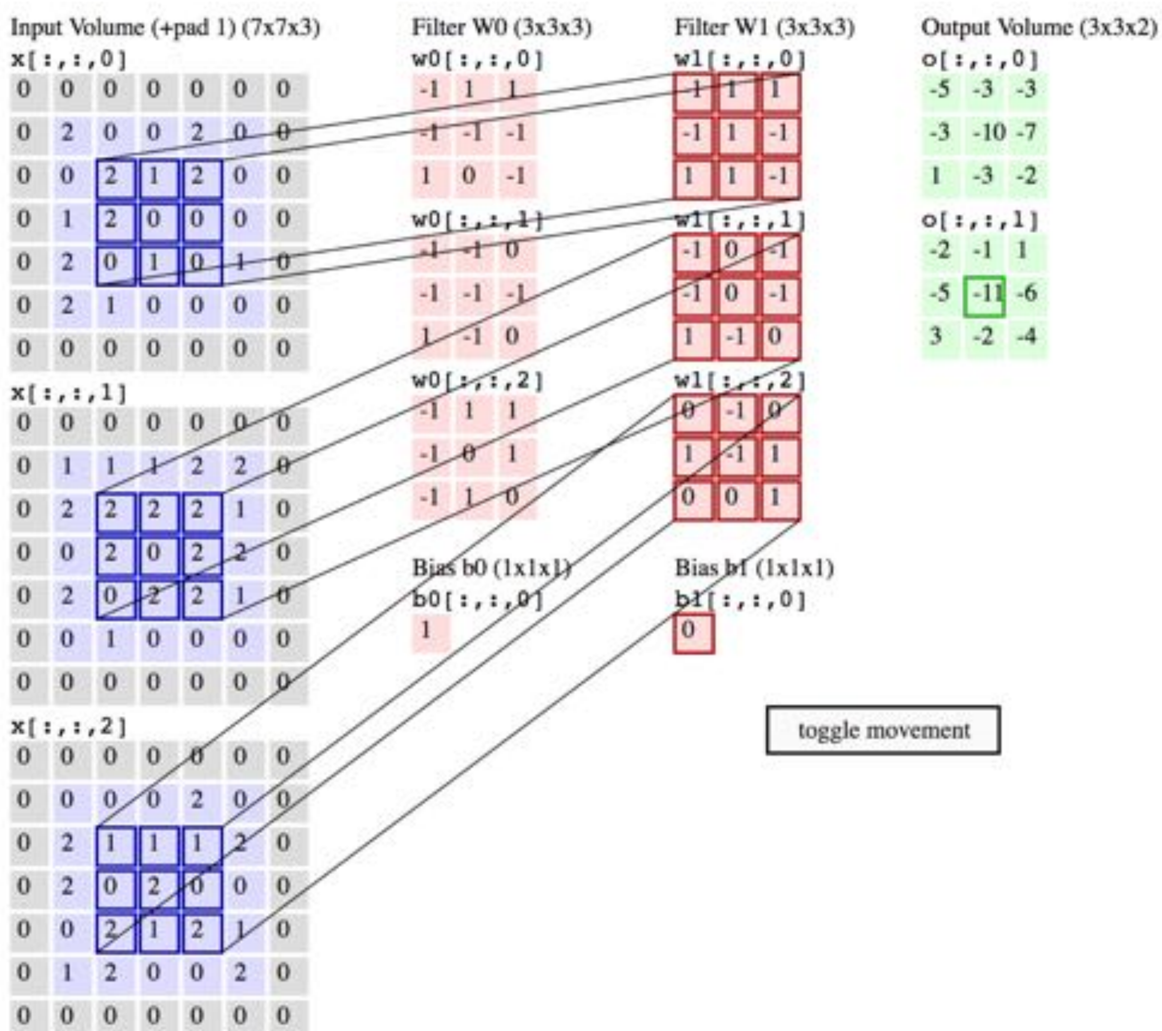


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

MNIST Digit Recognition with CNNs (in your browser)

https://cs.stanford.edu/people/karpathy/convnetjs/demo/mnist.html

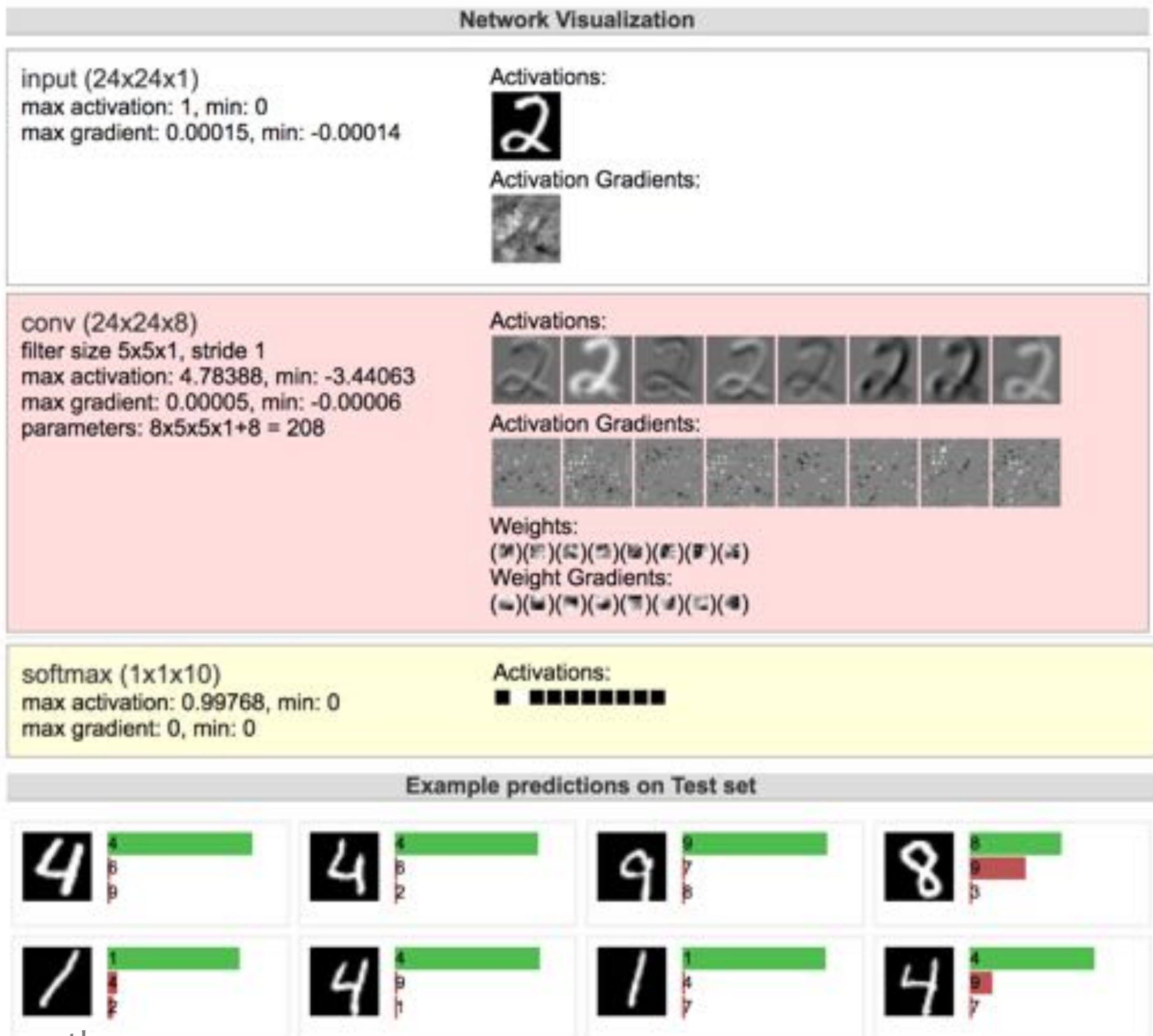


Figure from Andrej Karpathy

CNN Summary

CNNs

- Are used for all aspects of **computer vision**, and have won numerous pattern recognition competitions
- Able learn **interpretable features** at different levels of abstraction
- Typically, consist of **convolution** layers, **pooling** layers, **nonlinearities**, and **fully connected** layers

Other Resources:

- Readings on course website
- Andrej Karpathy, CS231n Notes http://cs231n.github.io/convolutional-networks/