10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Backpropagation
+
Deep Learning

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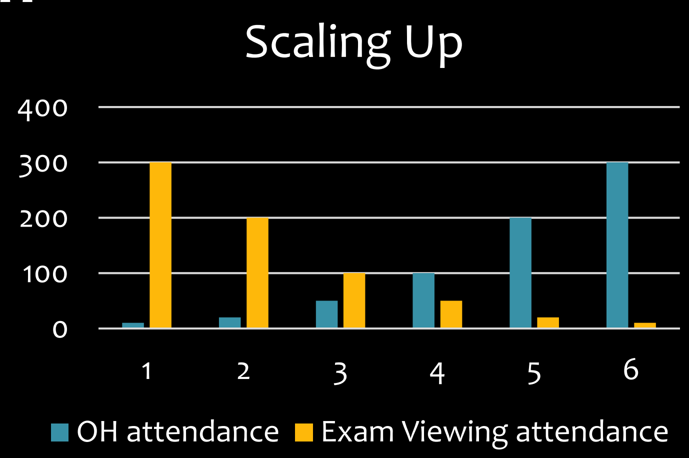
Lecture 14
Feb. 28, 2020

Reminders

- **Homework 4: Logistic Regression**
  - Out: Wed, Feb. 19
  - Due: Fri, Feb. 28 at 11:59pm
- **Homework 5: Neural Networks**
  - Out: Fri, Feb. 28
  - Due: Wed, Mar. 18 at 11:59pm
- **Today's In-Class Poll**
  - http://poll.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 (columns) / *Denominator* (rows)

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

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	$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x}\right]$	$\frac{\partial \mathbf{y}}{\partial x} = \left[\frac{\partial y_1}{\partial x} \quad \frac{\partial y_2}{\partial x} \quad \cdots \quad \frac{\partial y_N}{\partial x}\right]$
vector	$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_P} \end{bmatrix}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_N}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_N}{\partial x_2} \\ \vdots & & & \\ \frac{\partial y_1}{\partial x_P} & \frac{\partial y_2}{\partial x_P} & \cdots & \frac{\partial y_N}{\partial x_P} \end{bmatrix}$

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

$f(x)$	→	$\frac{\partial f}{\partial x}$
bx	→	b
xb	→	b
x^2	→	$2x$
bx^2	→	$2bx$

Vector Derivative

$f(x)$	→	$\frac{\partial f}{\partial \vec{x}}$
~~xB~~	~~→~~	~~B~~
$x^T b$	→	b
$x^T x$	→	$2x$
$x^T B x$	→	$2Bx$

↑ B symmetric

Not poll

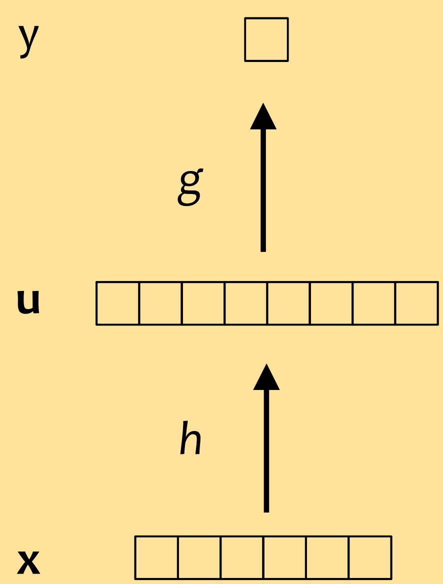
Matrix Calculus

Recall:

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

Question:

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



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

Answer:

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

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

Training

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**.

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

Training

Backpropagation

Chalkboard

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

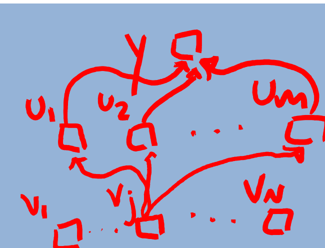
Training — Backpropagation

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 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

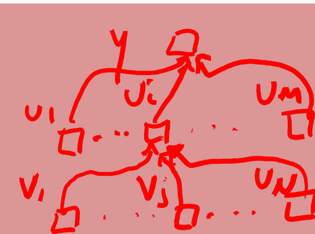
Automatic Differentiation – Reverse Mode (aka. Backpropagation)

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:

$$\left.\begin{aligned} \mathbf{g}_{\boldsymbol{\alpha}} &= \nabla_{\boldsymbol{\alpha}} J \\ \mathbf{g}_{\boldsymbol{\beta}} &= \nabla_{\boldsymbol{\beta}} J \end{aligned}\right\} = \text{NNBACKWARD}(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{o})$$

      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 $\boldsymbol{\alpha}, \boldsymbol{\beta}$

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

$$J = cos(u)$$

$$u = u_1 + u_2$$

$$u_1 = sin(t)$$

$$u_2 = 3t$$

$$t = x^2$$

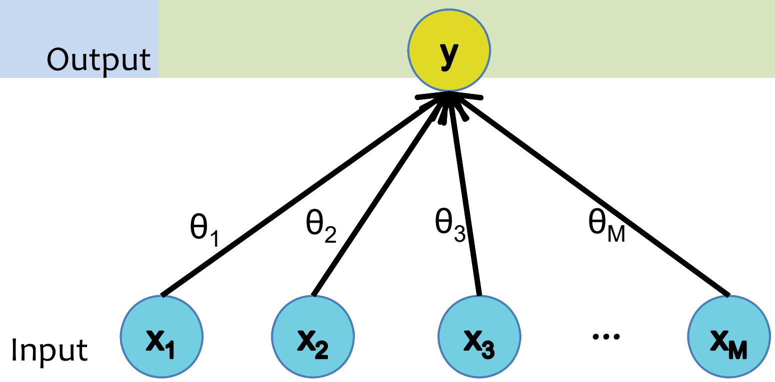
Training — Backpropagation

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

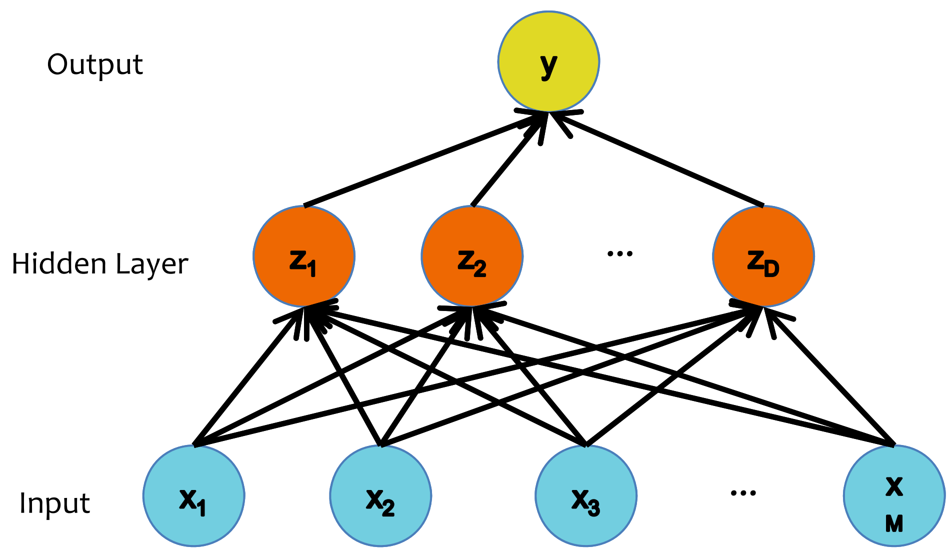
Backpropagation

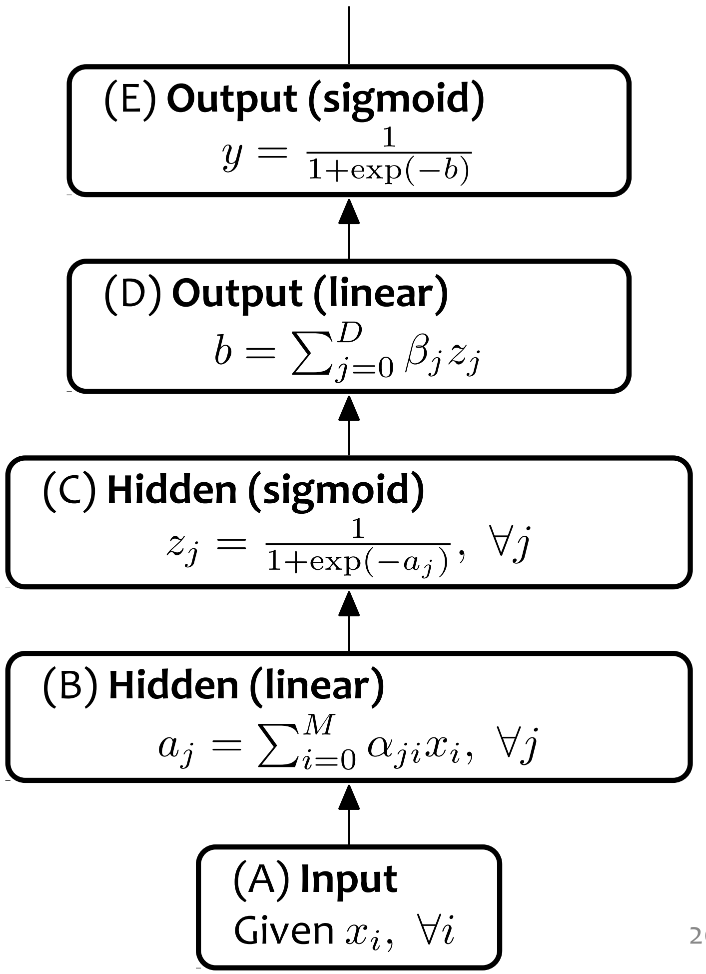
Case 1: Logistic Regression



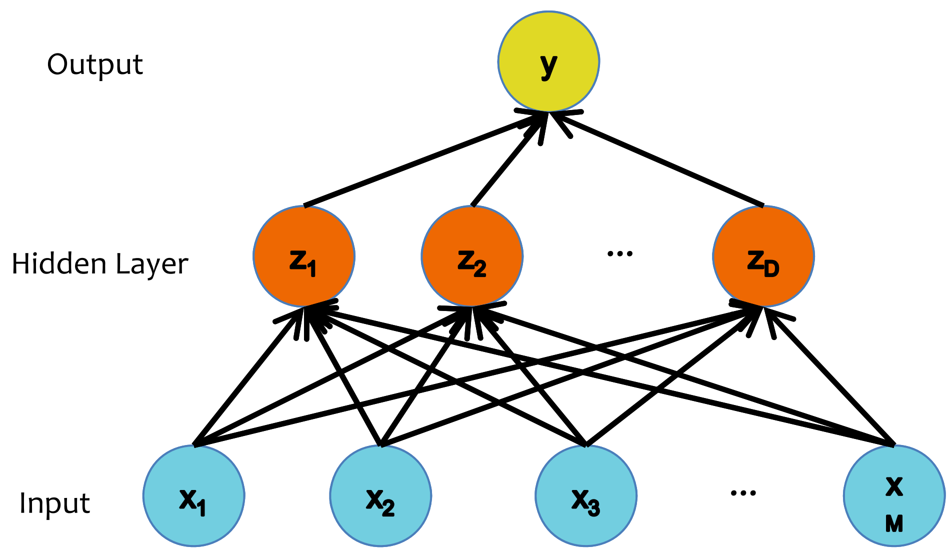
Forward	Backward
$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
$y = \frac{1}{1 + \exp(-a)}$	$\frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da}, \quad \frac{dy}{da} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$
$a = \sum_{j=0}^{D} \theta_j x_j$	$\frac{dJ}{d\theta_j}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

Training Backpropagation





Training Backpropagation



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

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

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

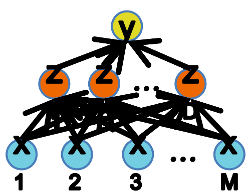
(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

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

Derivative of a Sigmoid

First suppose that

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

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

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

$$= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1 + 1 - 1)^2} \quad (3)$$

$$= \frac{\exp(-b) + 1 - 1}{(\exp(-b) + 1)^2} \quad (4)$$

$$= \frac{\exp(-b) + 1}{(\exp(-b) + 1)^2} - \frac{1}{(\exp(-b) + 1)^2} \quad (5)$$

$$= \frac{1}{(\exp(-b) + 1)} - \frac{1}{(\exp(-b) + 1)^2} \quad (6)$$

$$= \frac{1}{(\exp(-b) + 1)} - \left(\frac{1}{(\exp(-b) + 1)} \frac{1}{(\exp(-b) + 1)}\right) \quad (7)$$

$$= \frac{1}{(\exp(-b) + 1)} \left(1 - \frac{1}{(\exp(-b) + 1)}\right) \quad (8)$$

$$= s(1 - s) \quad (9)$$

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

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

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

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
   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(**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

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 $\boldsymbol{\alpha}, \boldsymbol{\beta}$

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!

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

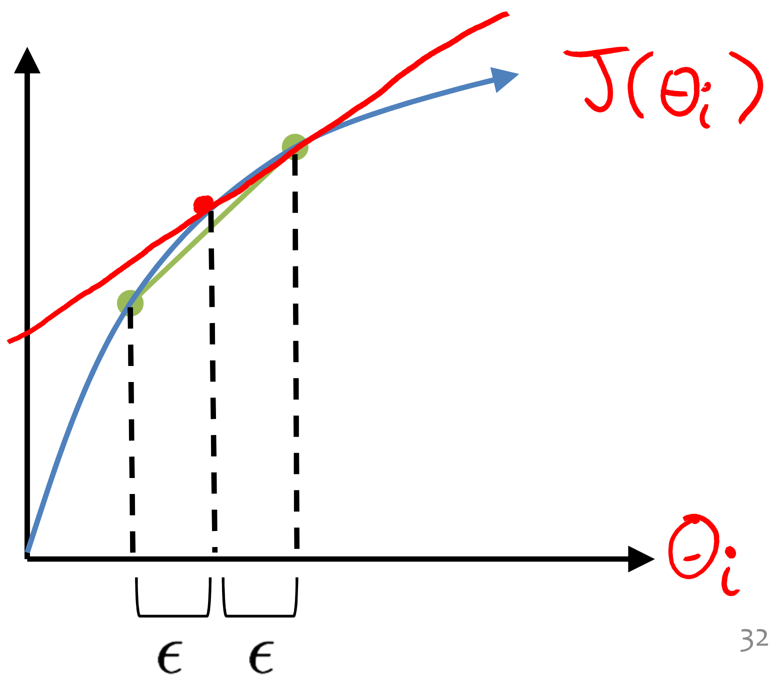
OTHER APPROACHES TO DIFFERENTIATION

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

Training

Differentiation Quiz

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**.

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

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

A. ~~[4.2, -7.2]~~
B. [7.2, -4.2]
C. [1.10, 2.7]
D. [2.7, 1.10]
E. [8.1, 12.2]
F. [12.2, 8.1]
G. [-0.97, -1.28]
H. [-1.28, -0.97]

Symbolic Differentiation

Differentiation Quiz #2:

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

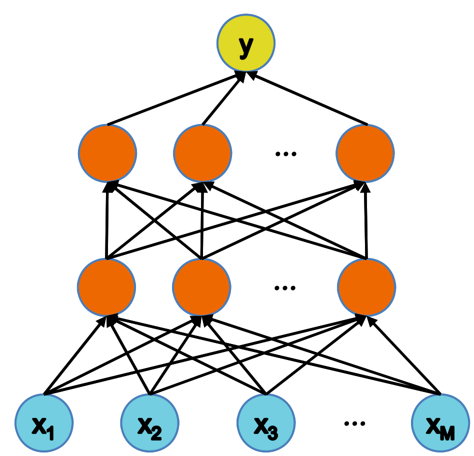
$$y = \sigma(\boldsymbol{\beta}^T \sigma((\boldsymbol{\alpha}^{(2)})^T \sigma((\boldsymbol{\alpha}^{(1)})^T \mathbf{x}))$$

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

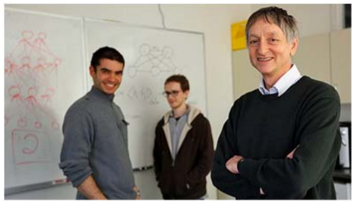
DEEP LEARNING

Deep Learning Outline

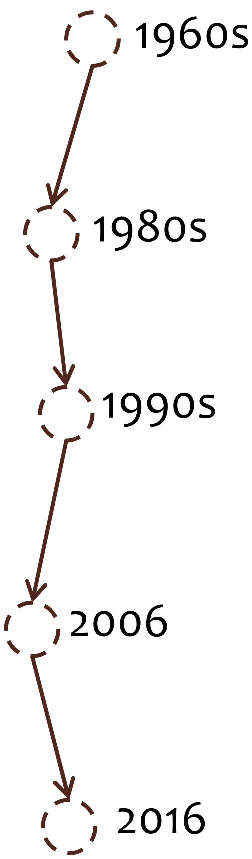
- **Background: Computer Vision**
  - Image Classification
  - ILSVRC 2010 - 2016
  - Traditional Feature Extraction Methods
  - Convolution as Feature Extraction
- **Convolutional Neural Networks (CNNs)**
  - Learning Feature Abstractions
  - Common CNN Layers:
    - Convolutional Layer
    - Max-Pooling 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!

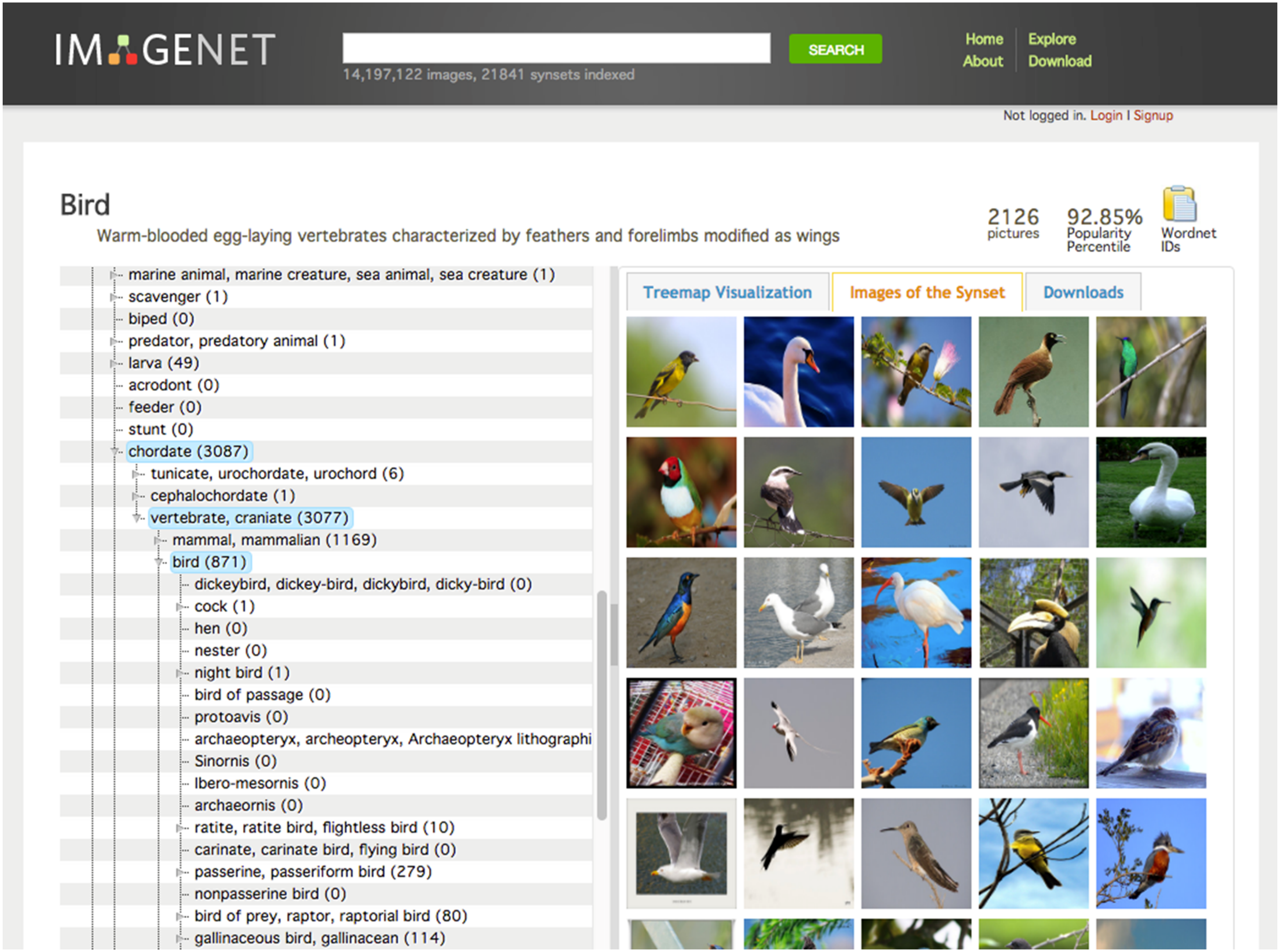
Since 1980s: Form of models hasn't changed much, but lots of new tricks…

- 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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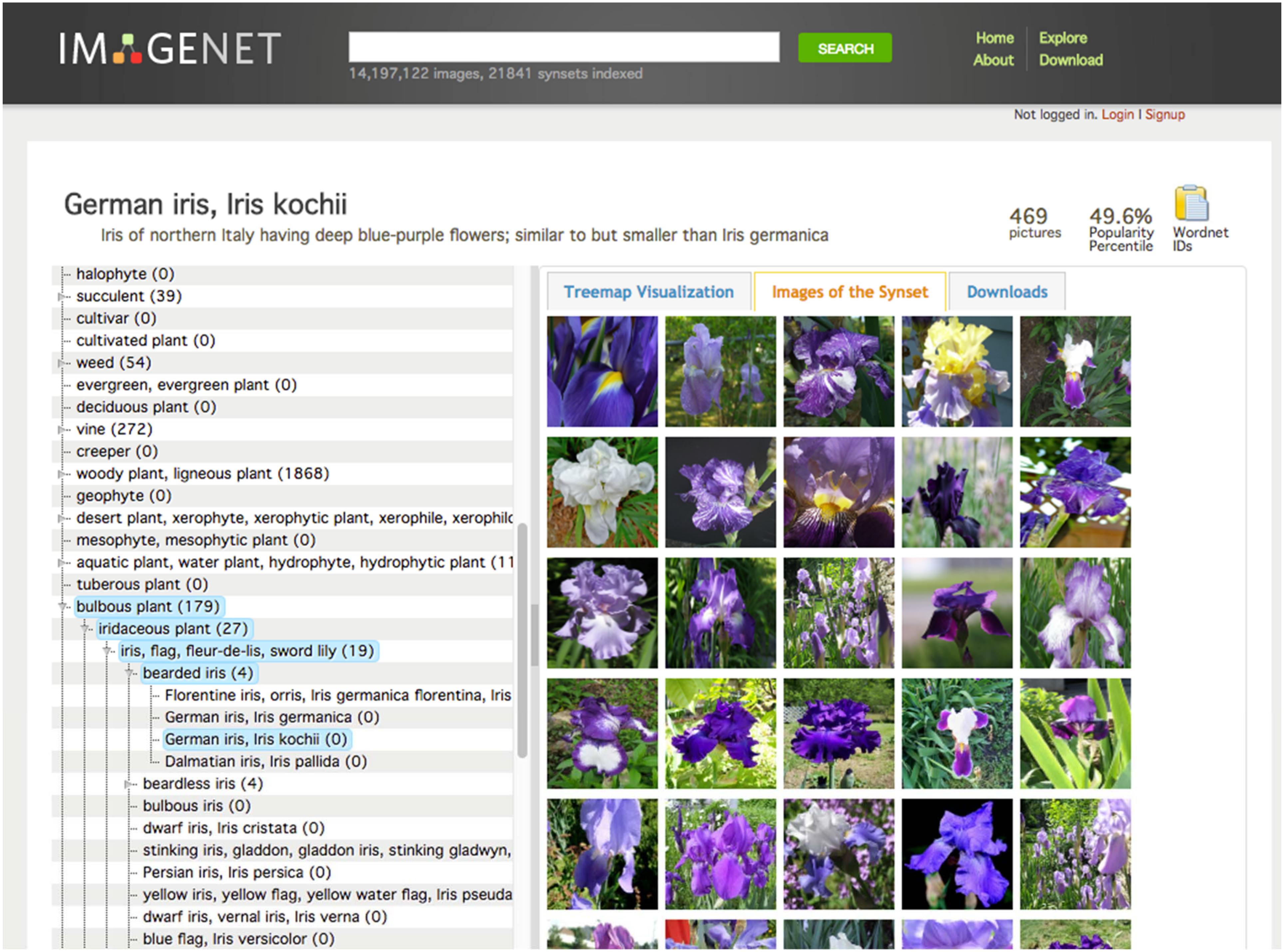
Bird
Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings
2126 pictures
92.85% Popularity Percentile
Wordnet IDs
marine animal, marine creature, sea animal, sea creature (1)
scavenger (1)
biped (0)
predator, predatory animal (1)
larva (49)
acrodont (0)
feeder (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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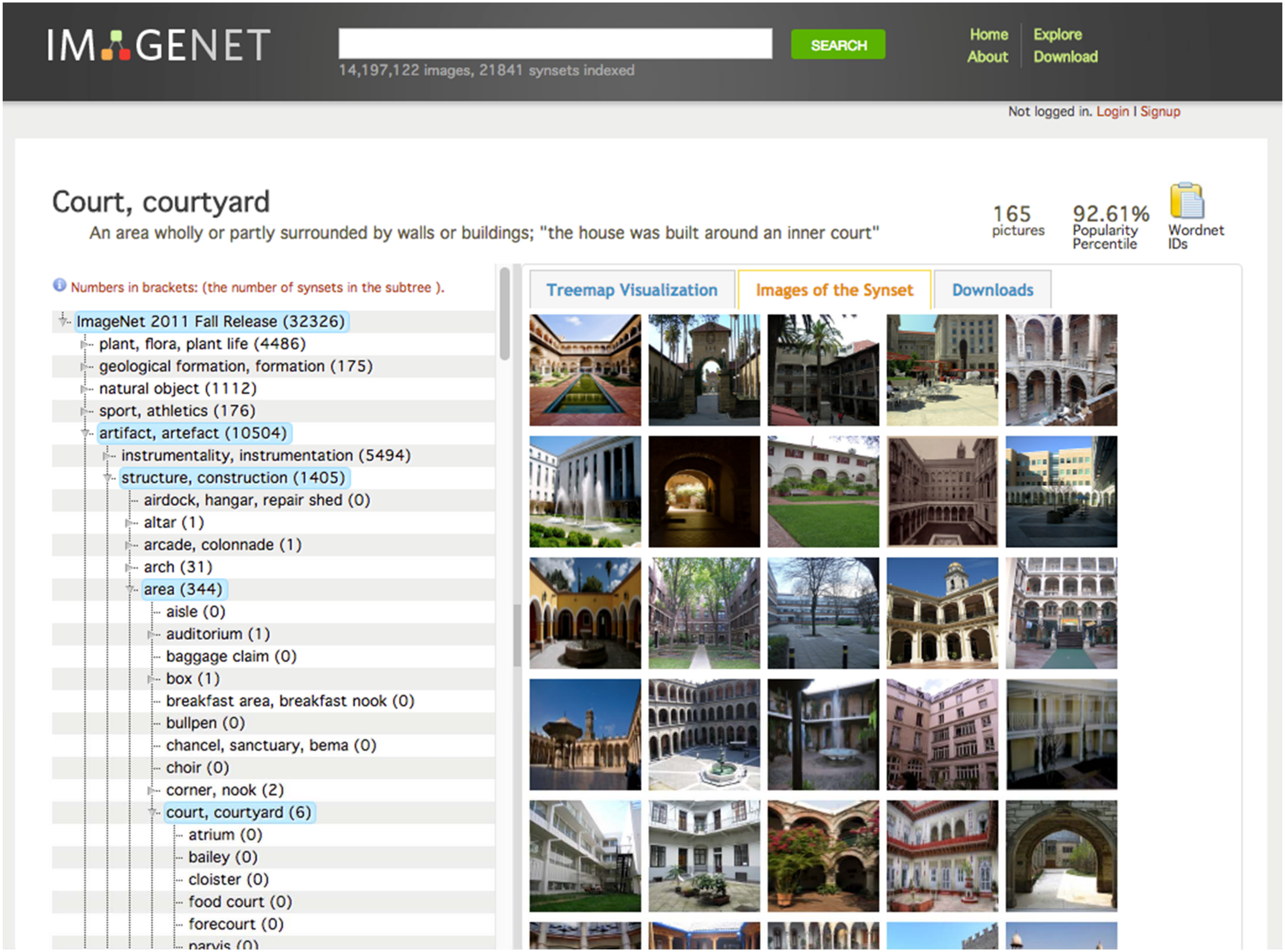
German iris, Iris kochii
Iris of northern Italy having deep blue-purple flowers; similar to but smaller than Iris germanica
469
pictures
49.6%
Popularity
Percentile
Wordnet
IDs
halophyte (0)
succulent (39)
cultivar (0)
cultivated plant (0)
weed (54)
evergreen, evergreen plant (0)
deciduous plant (0)
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


IMAGENET
SEARCH
14,197,122 images, 21841 synsets indexed
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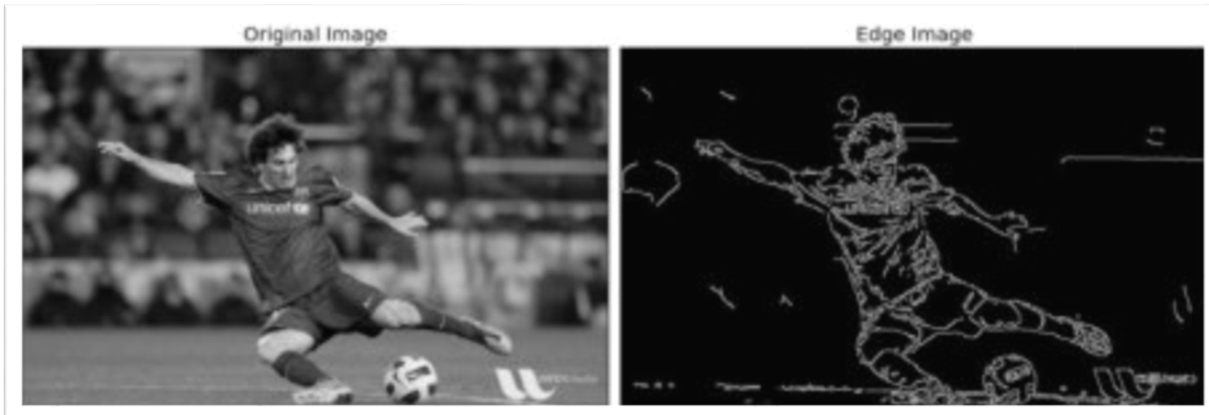
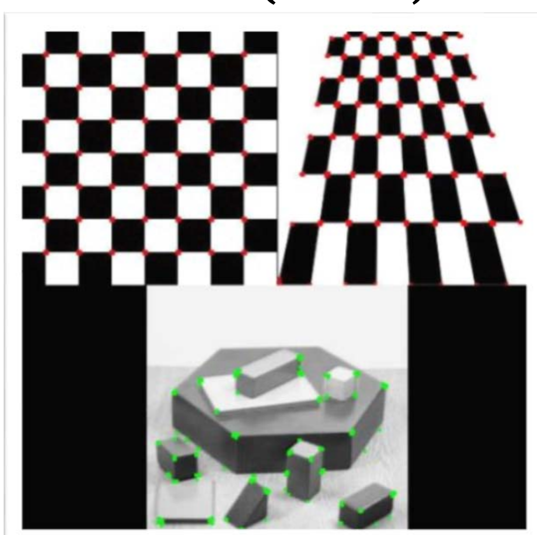
Court, courtyard
An area wholly or partly surrounded by walls or buildings; "the house was built around an inner court"
165 pictures
92.61% Popularity Percentile
Wordnet IDs
Numbers in brackets: (the number of synsets in the subtree).
ImageNet 2011 Fall Release (32326)
plant, flora, plant life (4486)
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)

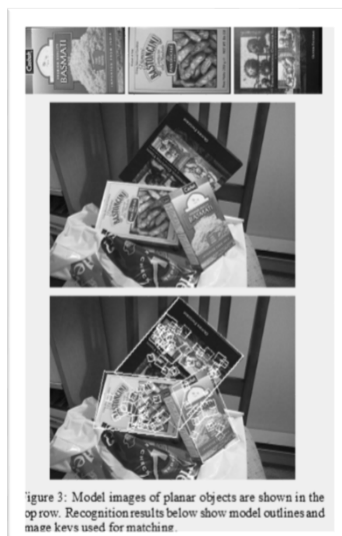


Corner Detection (Harris)



Figures from http://opencv.org

Scale Invariant Feature Transform (SIFT)



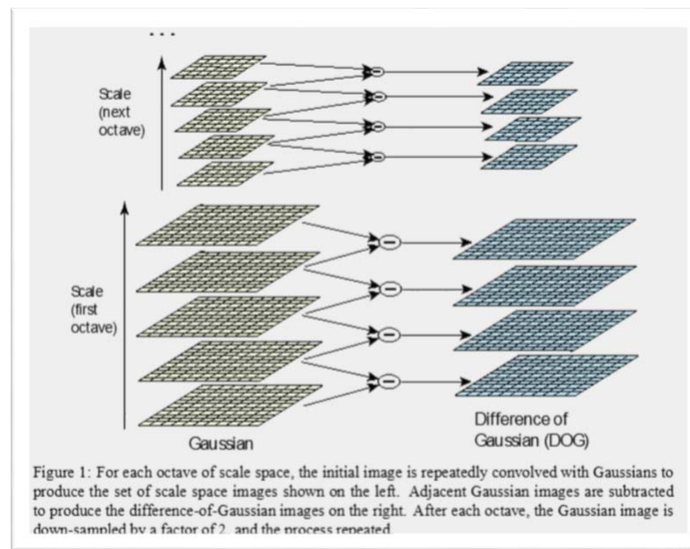


Figure from Lowe (1999) and Lowe (2004)

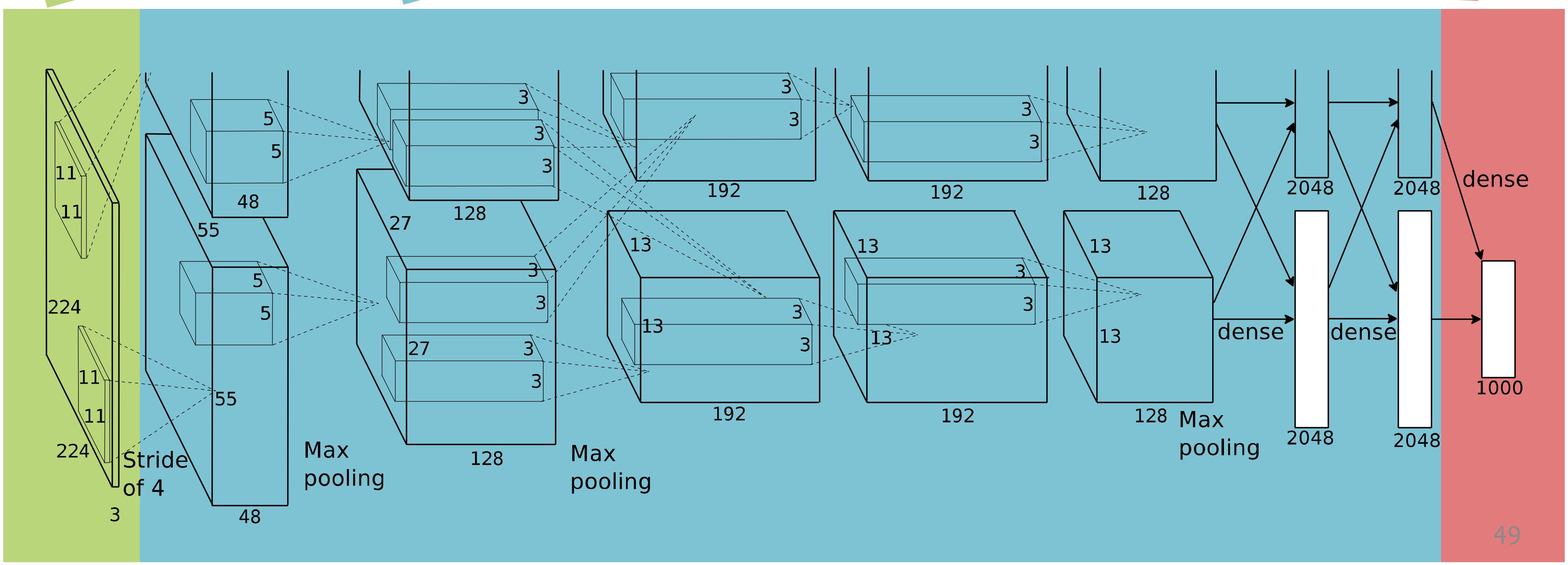
Example: Image Classification

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

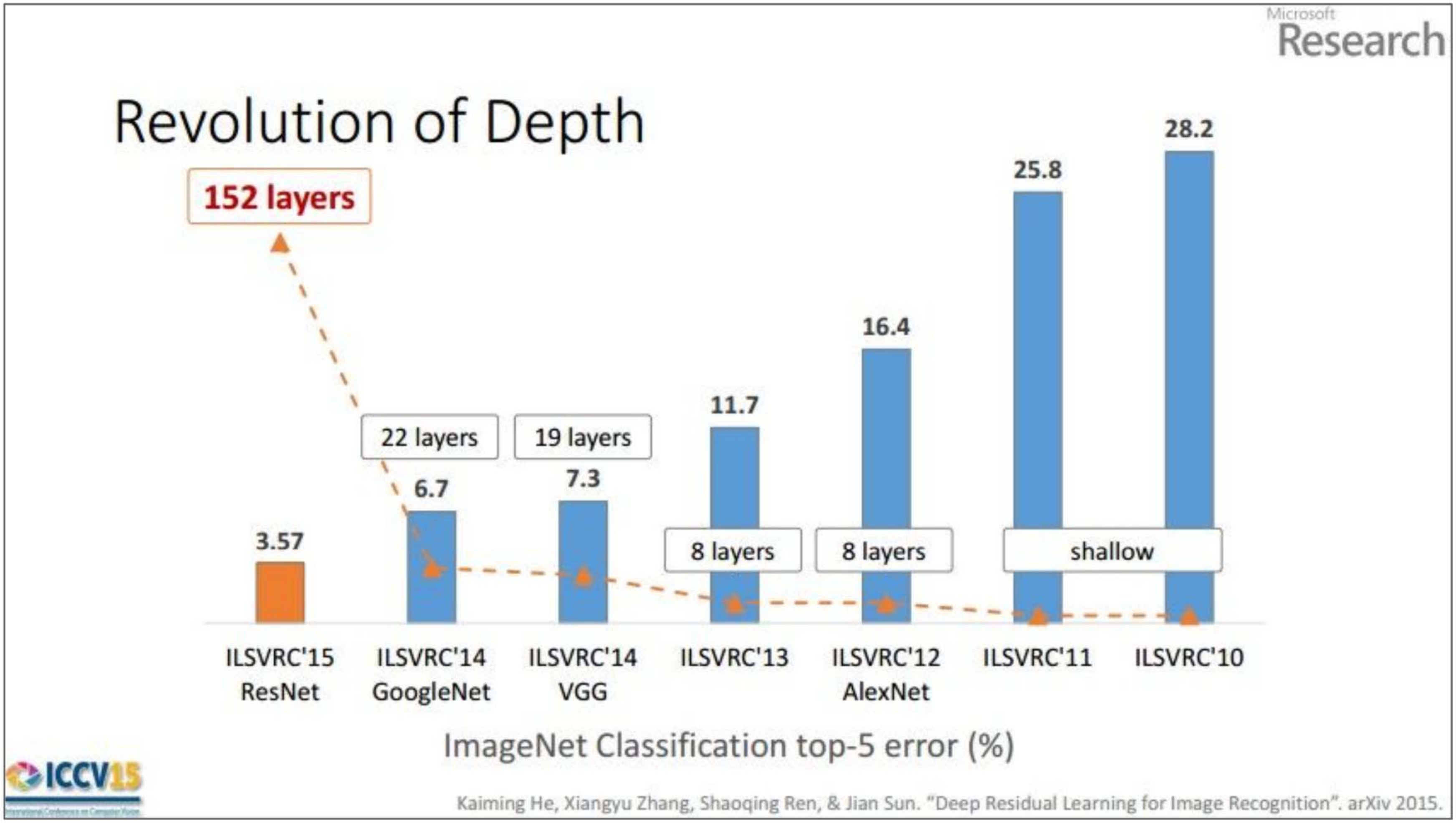
Input image (pixels)

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

1000-way softmax



CNNs for Image Recognition



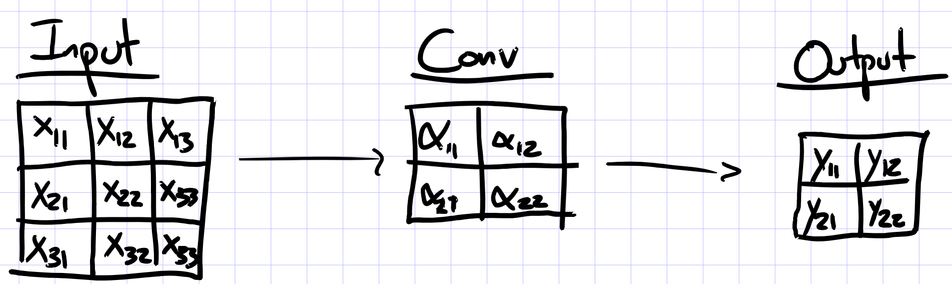
Slide from Kaiming He

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



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

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

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

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

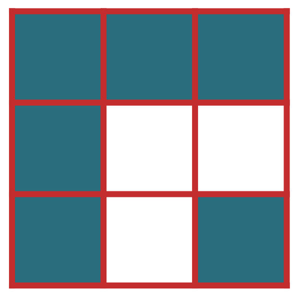
Background: Image Processing

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

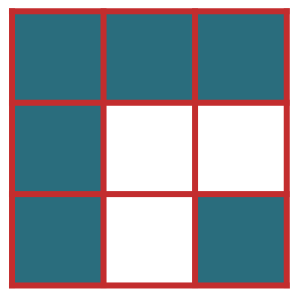
Background: Image Processing

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

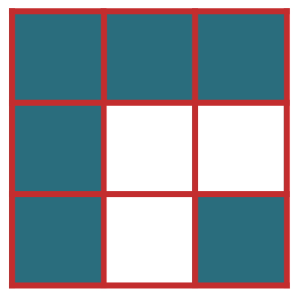
Background: Image Processing

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

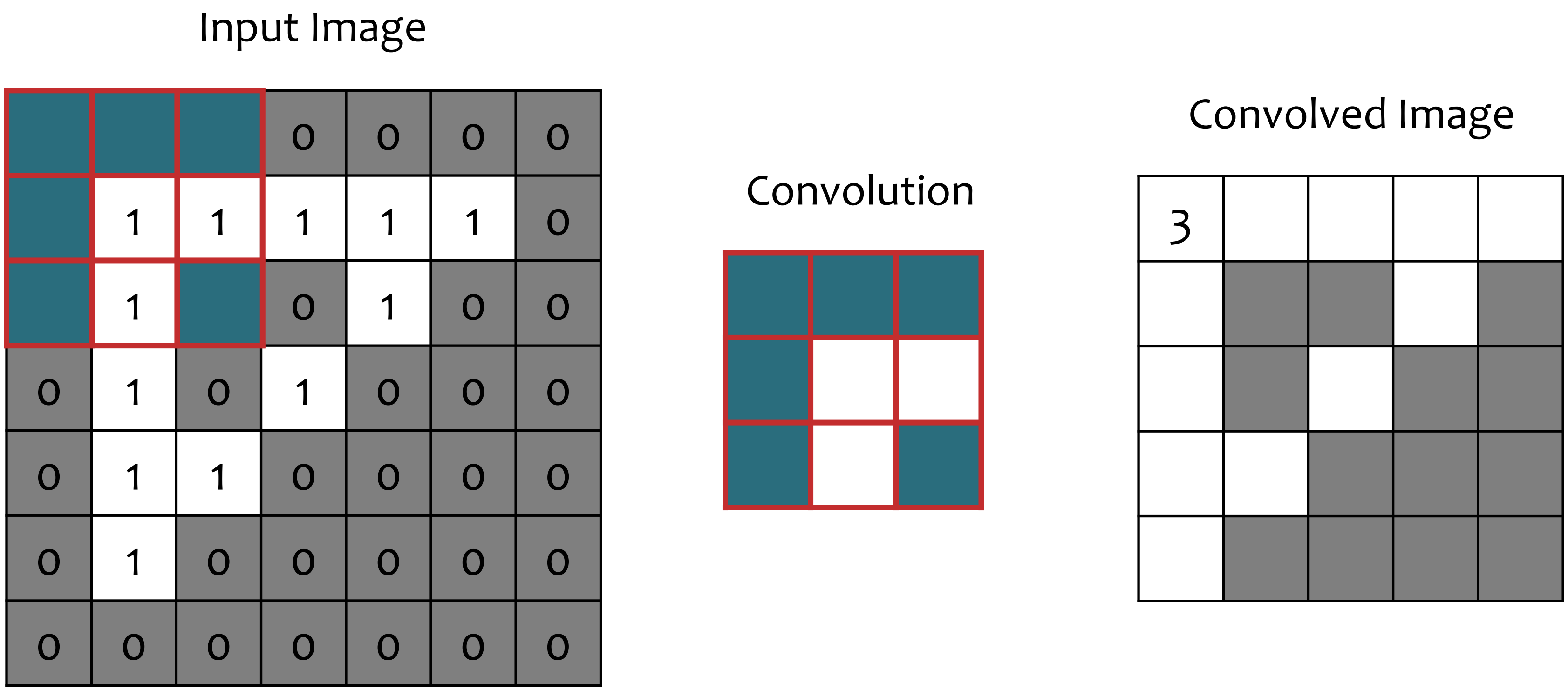


Convolved Image

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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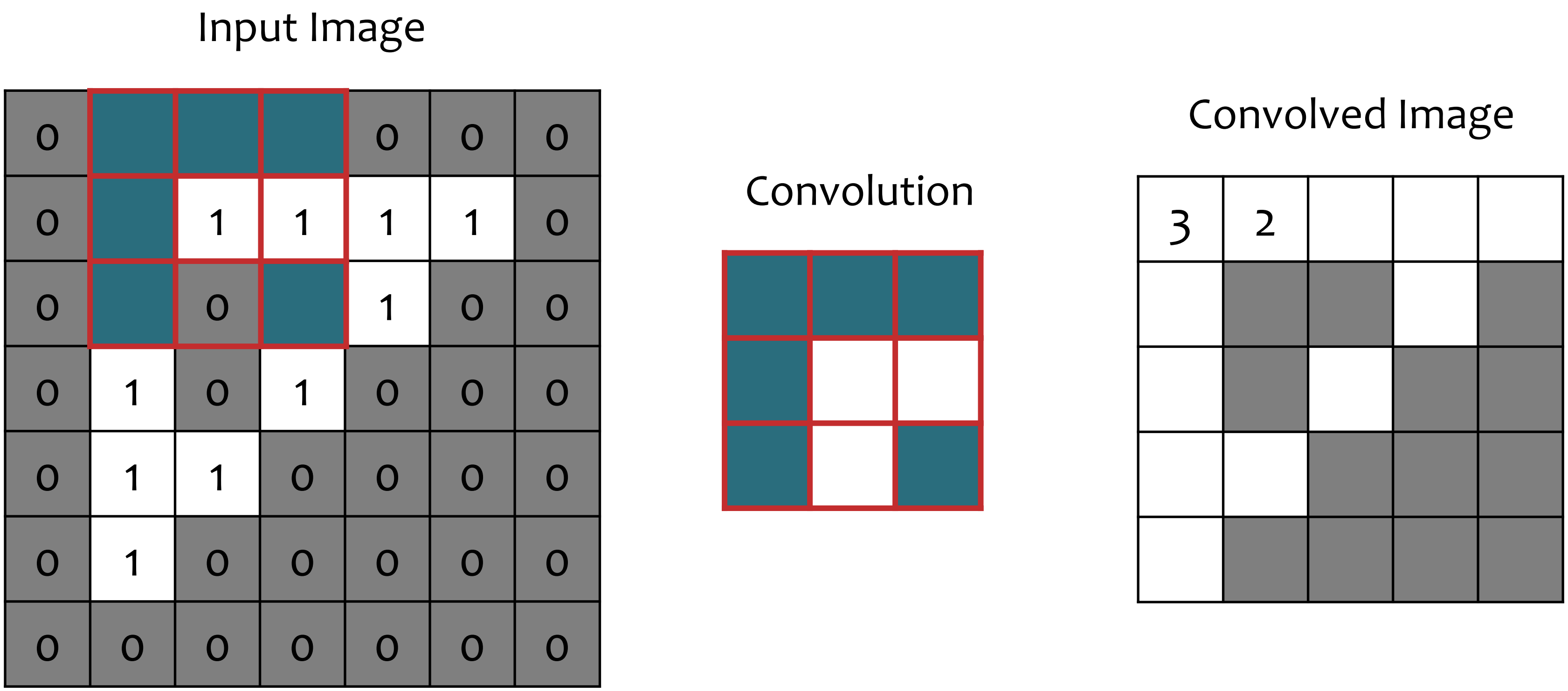

Background: Image Processing

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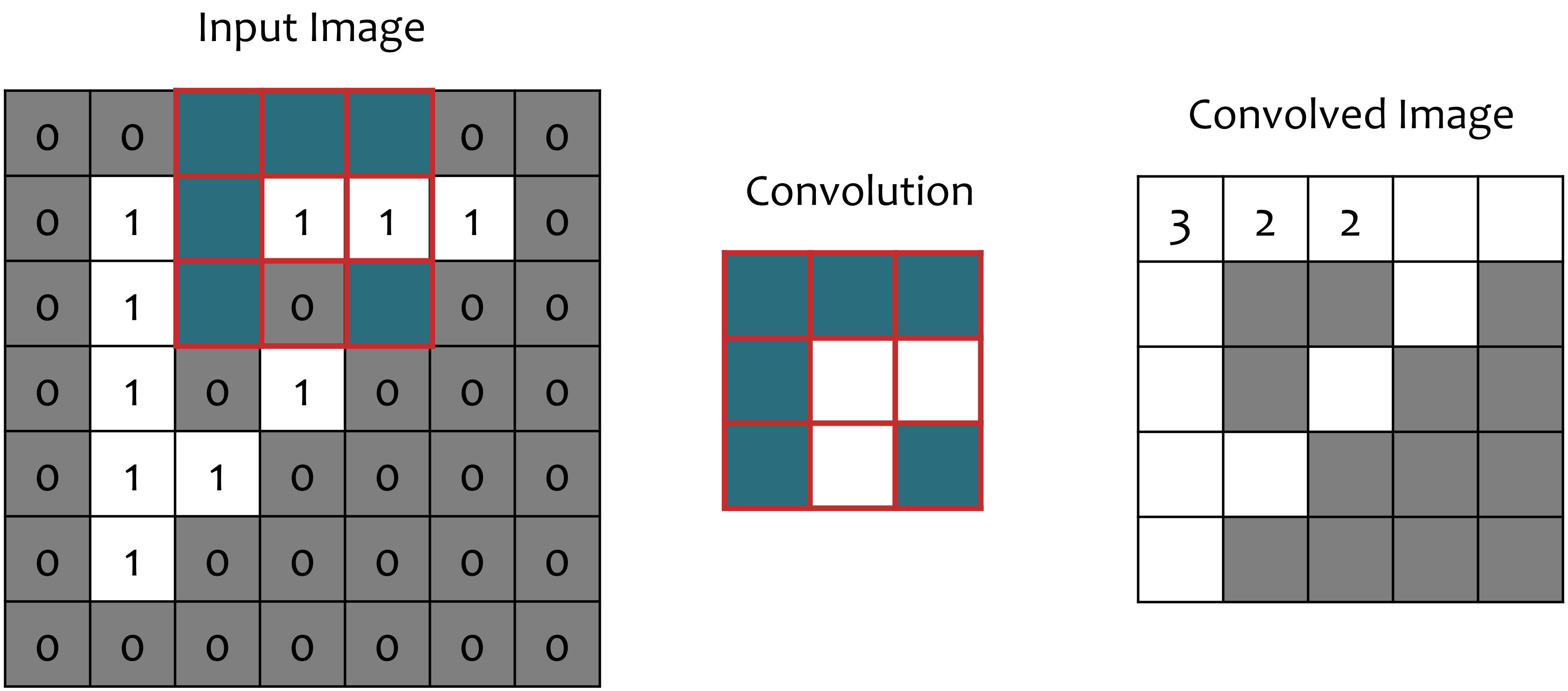

Background: Image Processing

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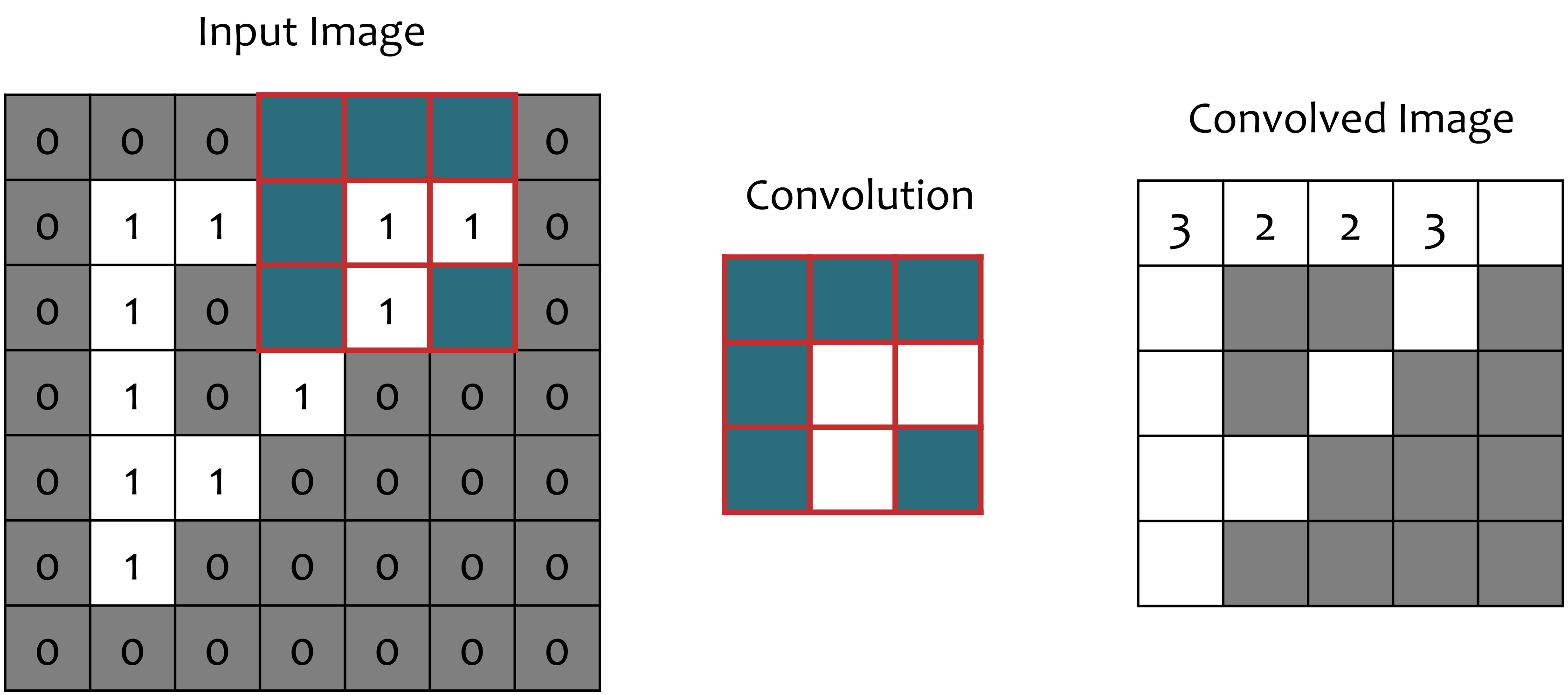
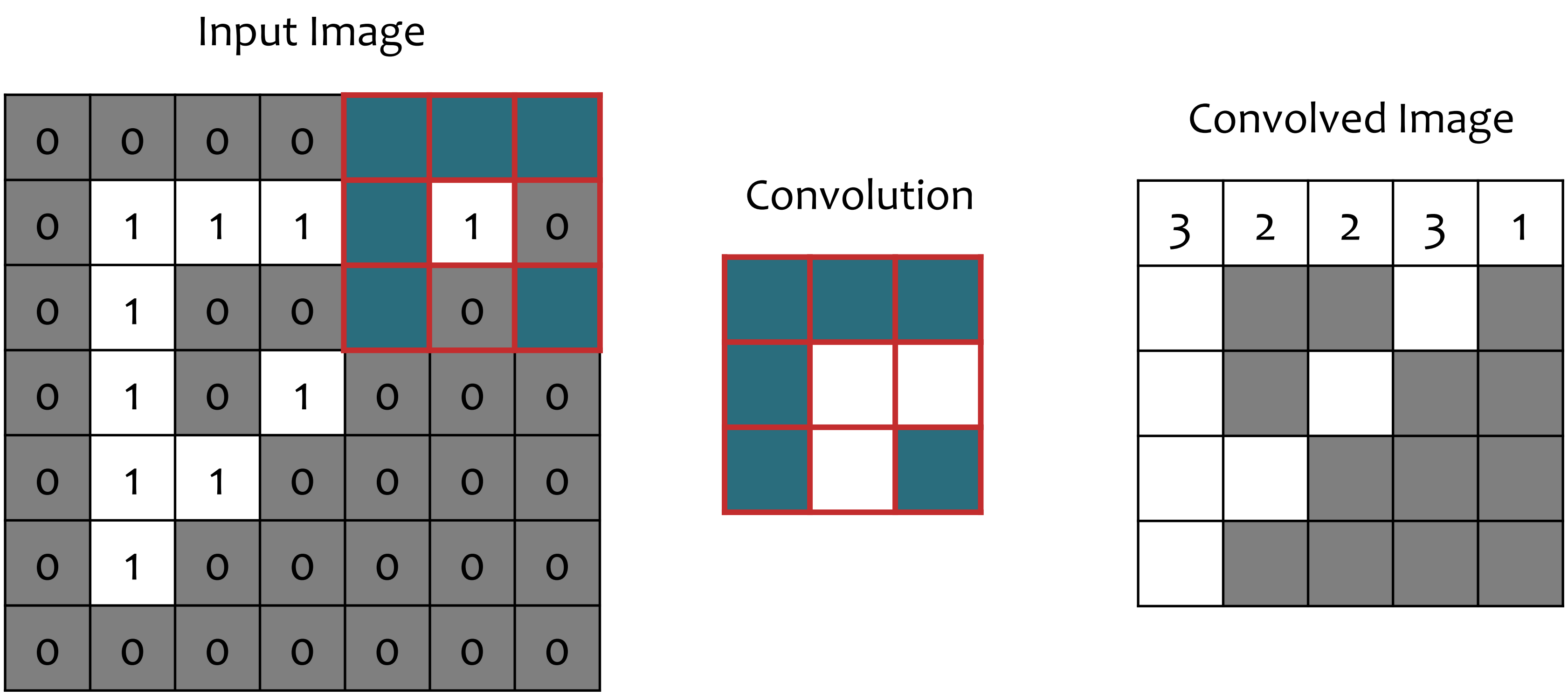


Background: Image Processing

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



Background: Image Processing

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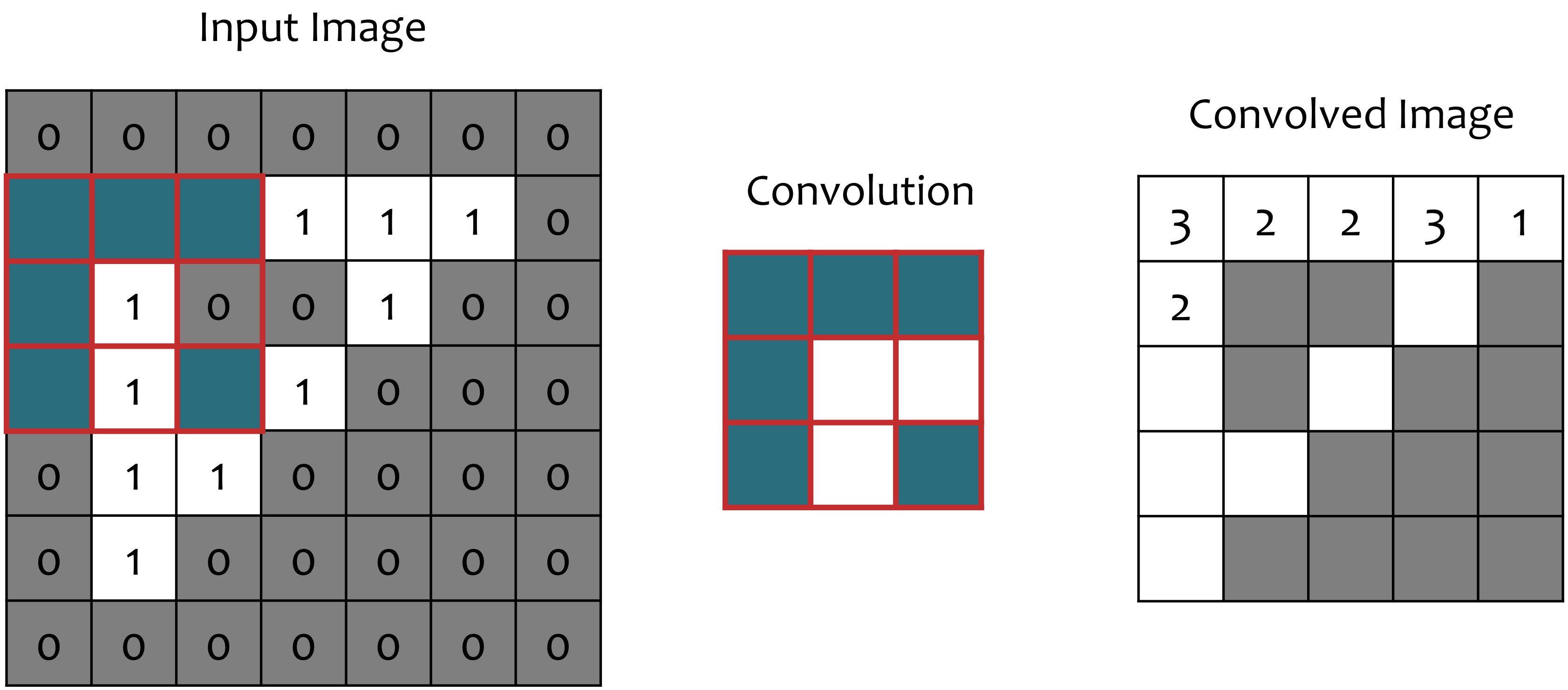
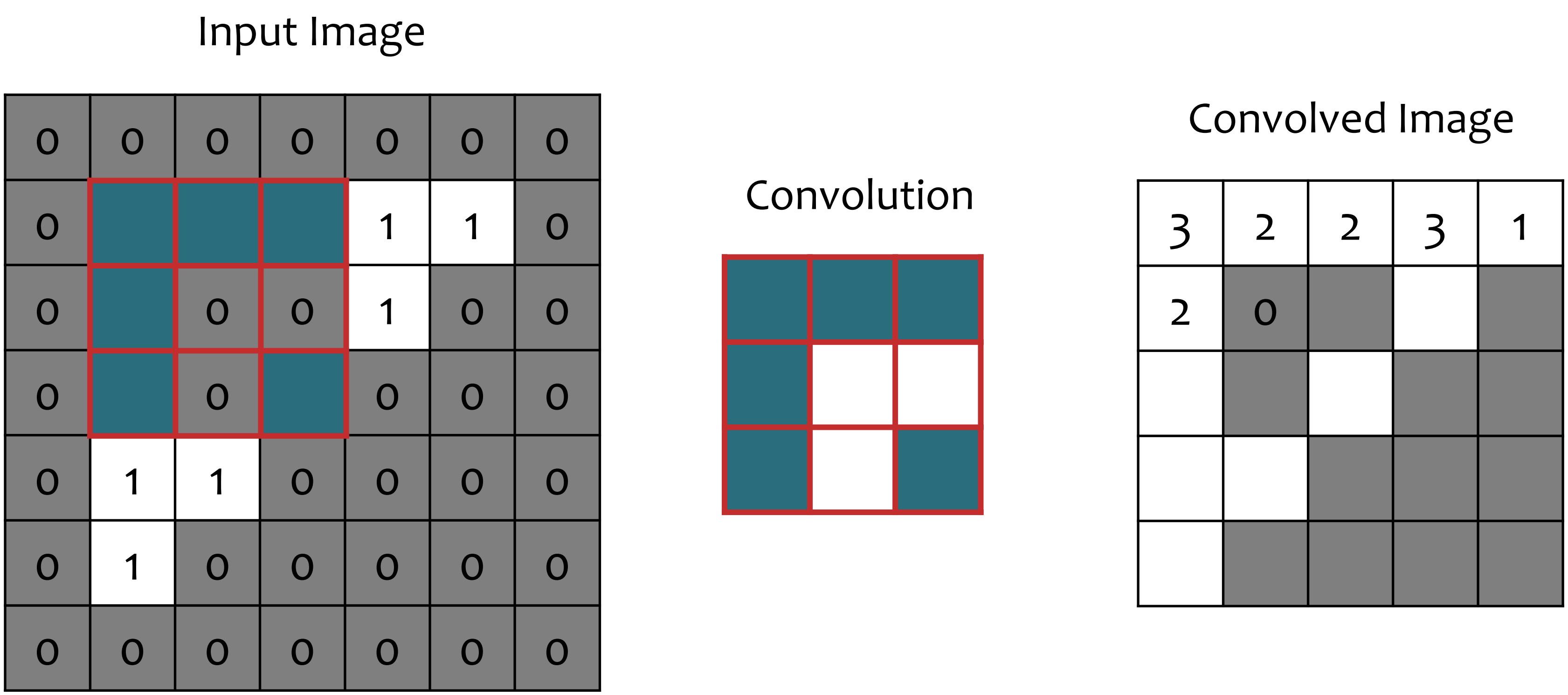


Background: Image Processing

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



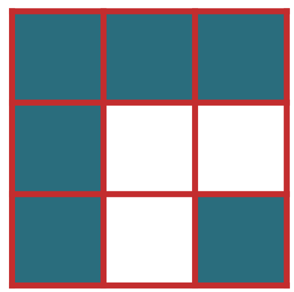
Background: Image Processing

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

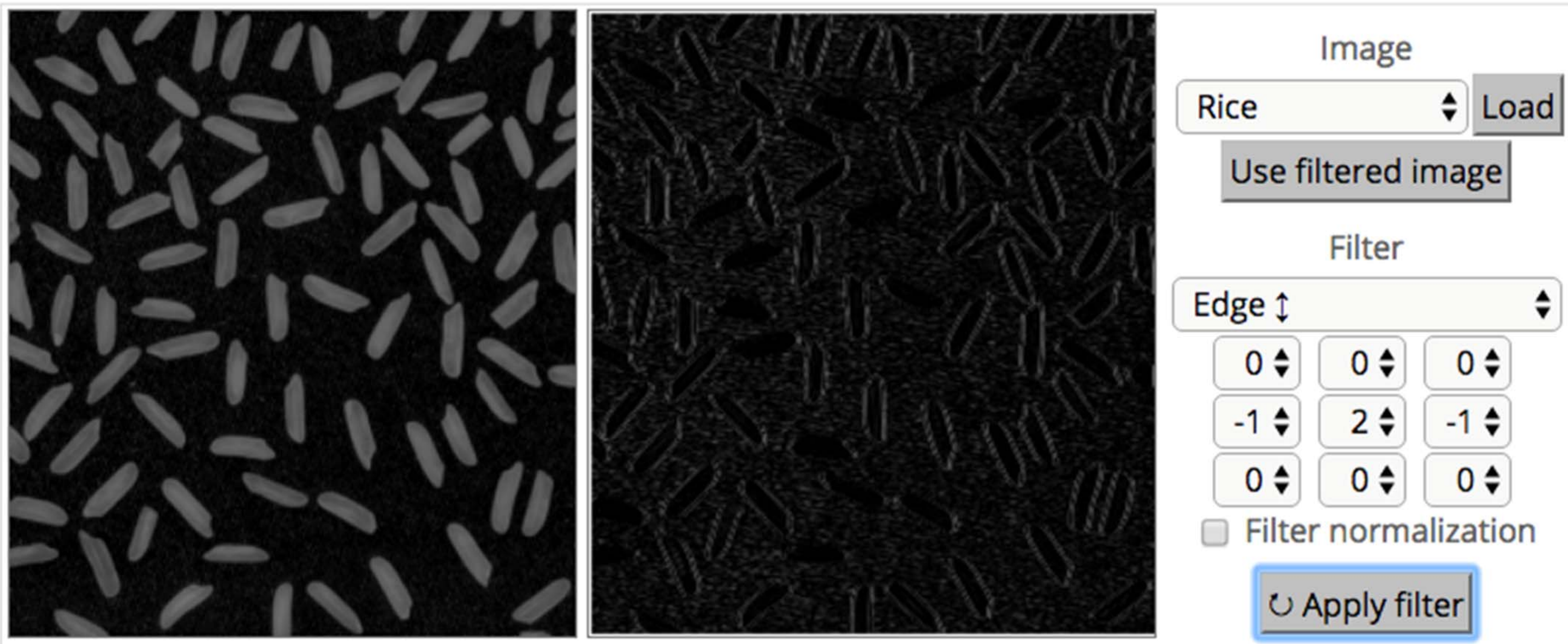
.1	.1	.1
.1	.2	.1
.1	.1	.1

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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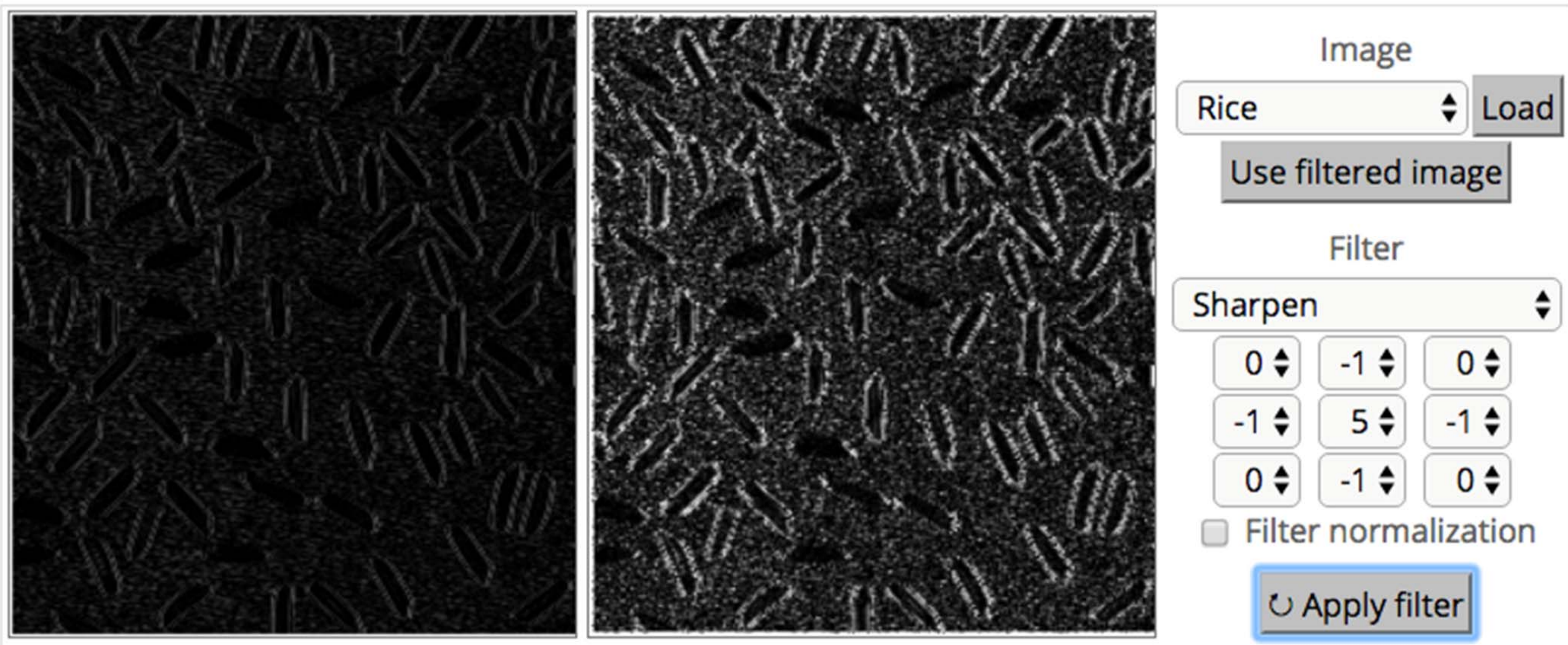

Slide from William Cohen

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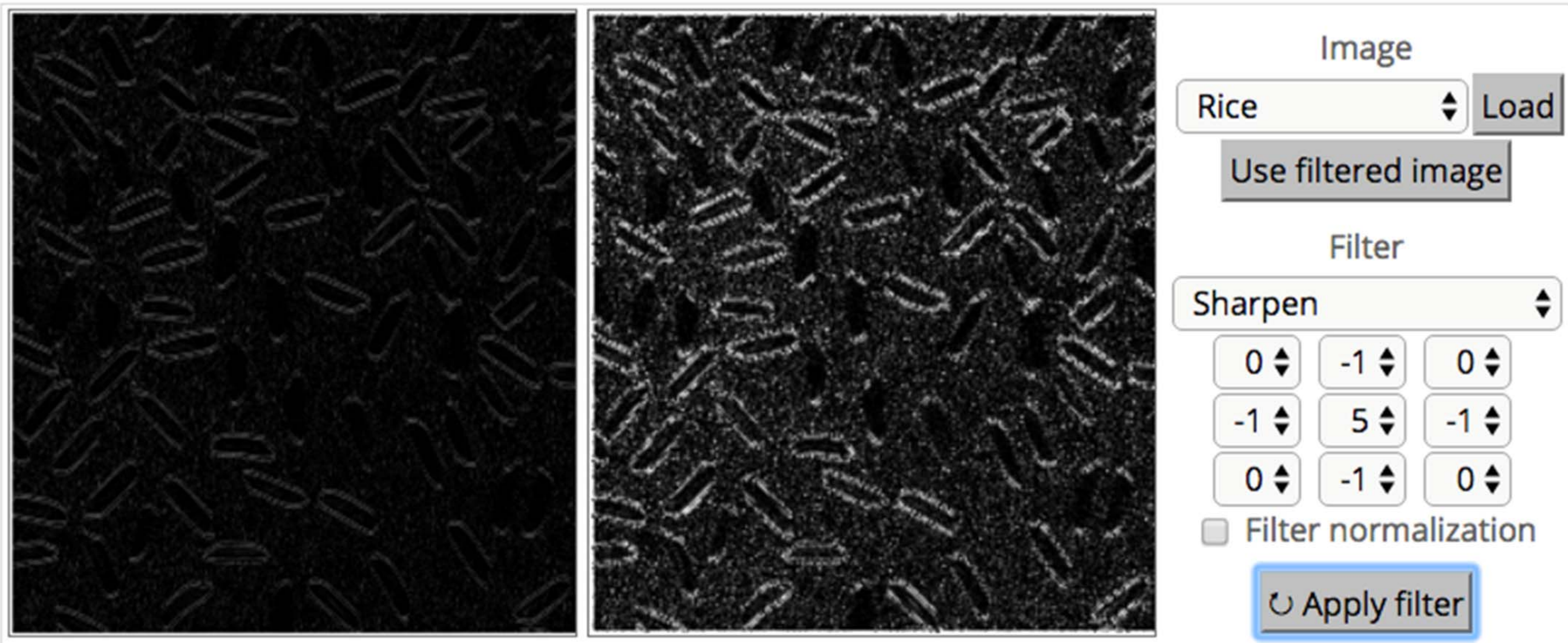

Slide from William Cohen

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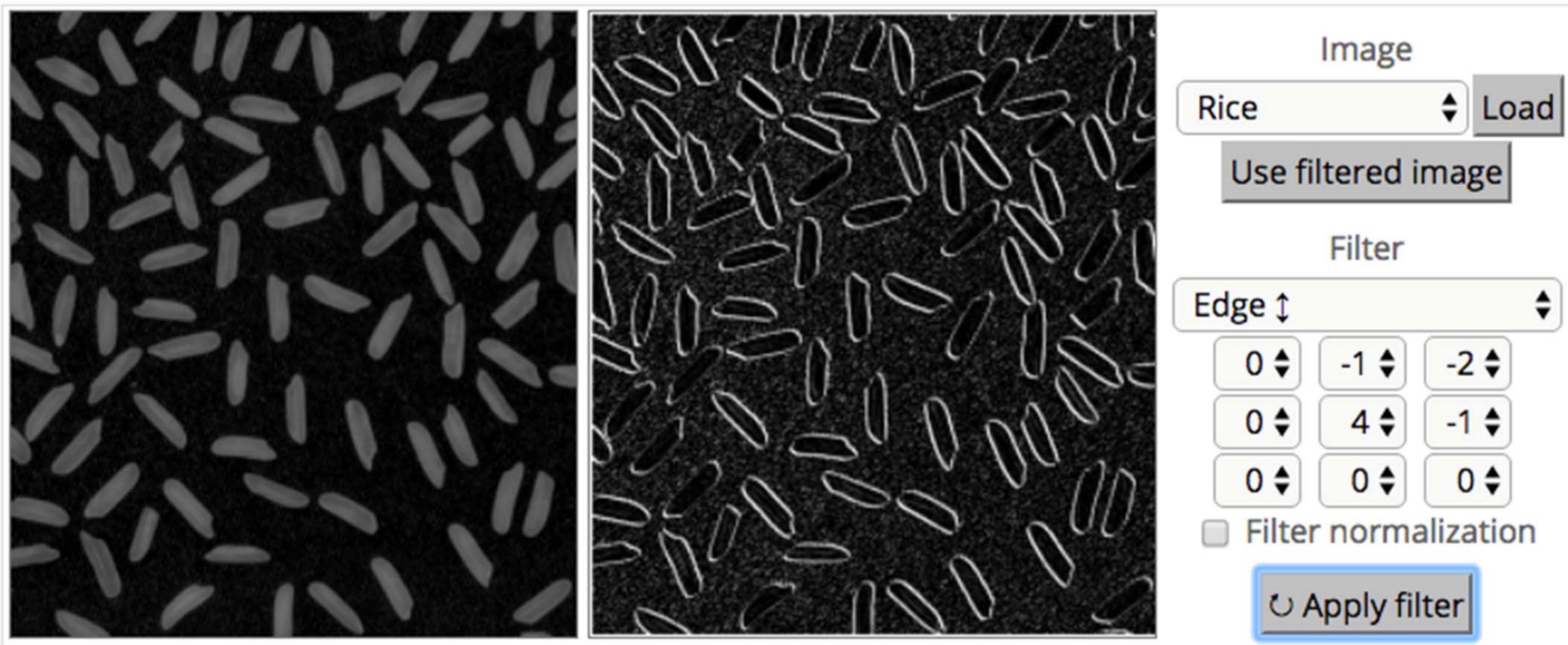

Slide from William Cohen

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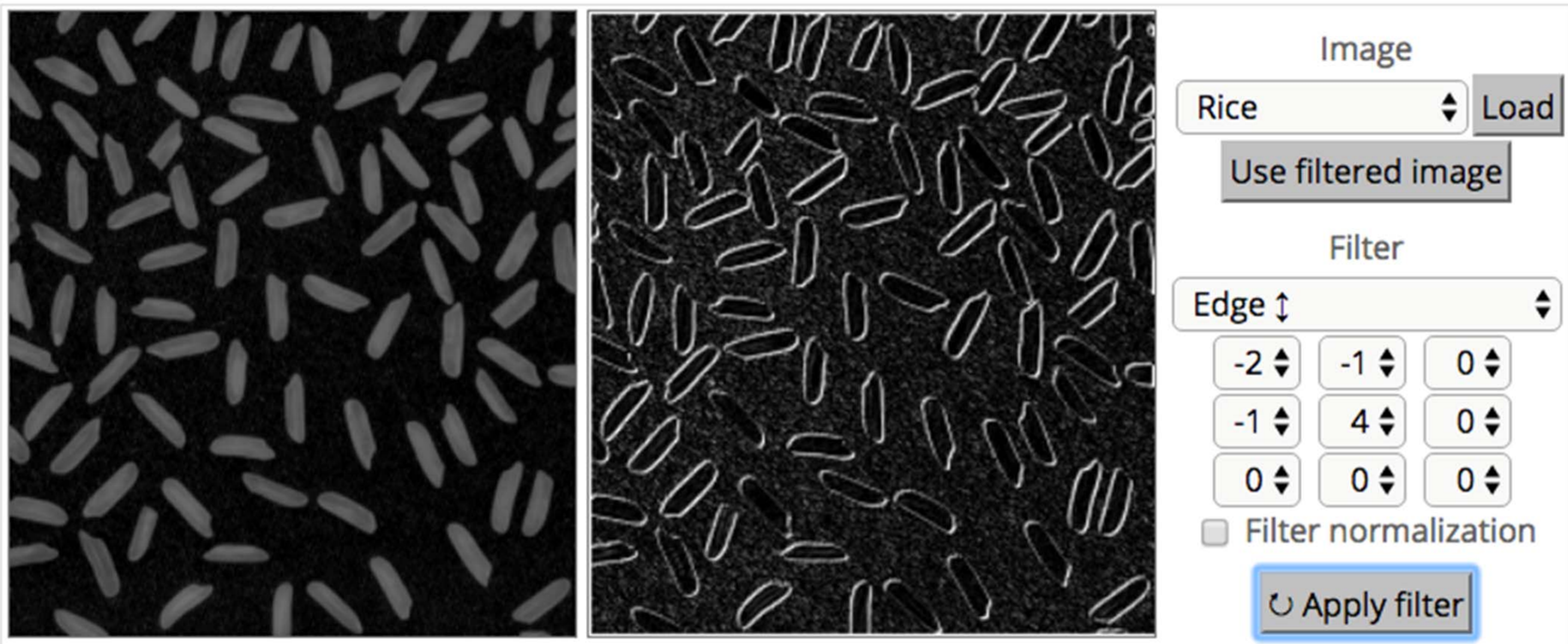
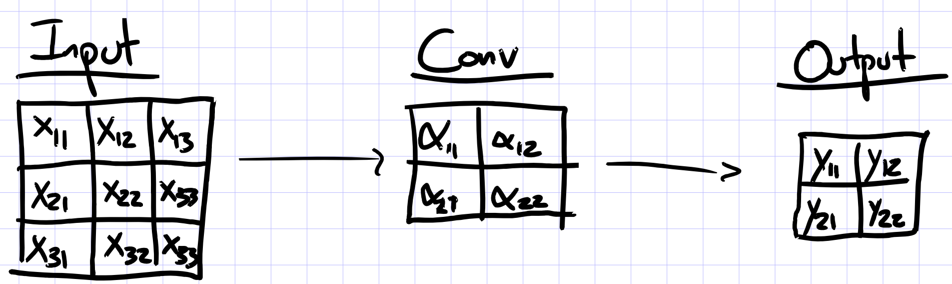


Slide from William Cohen

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



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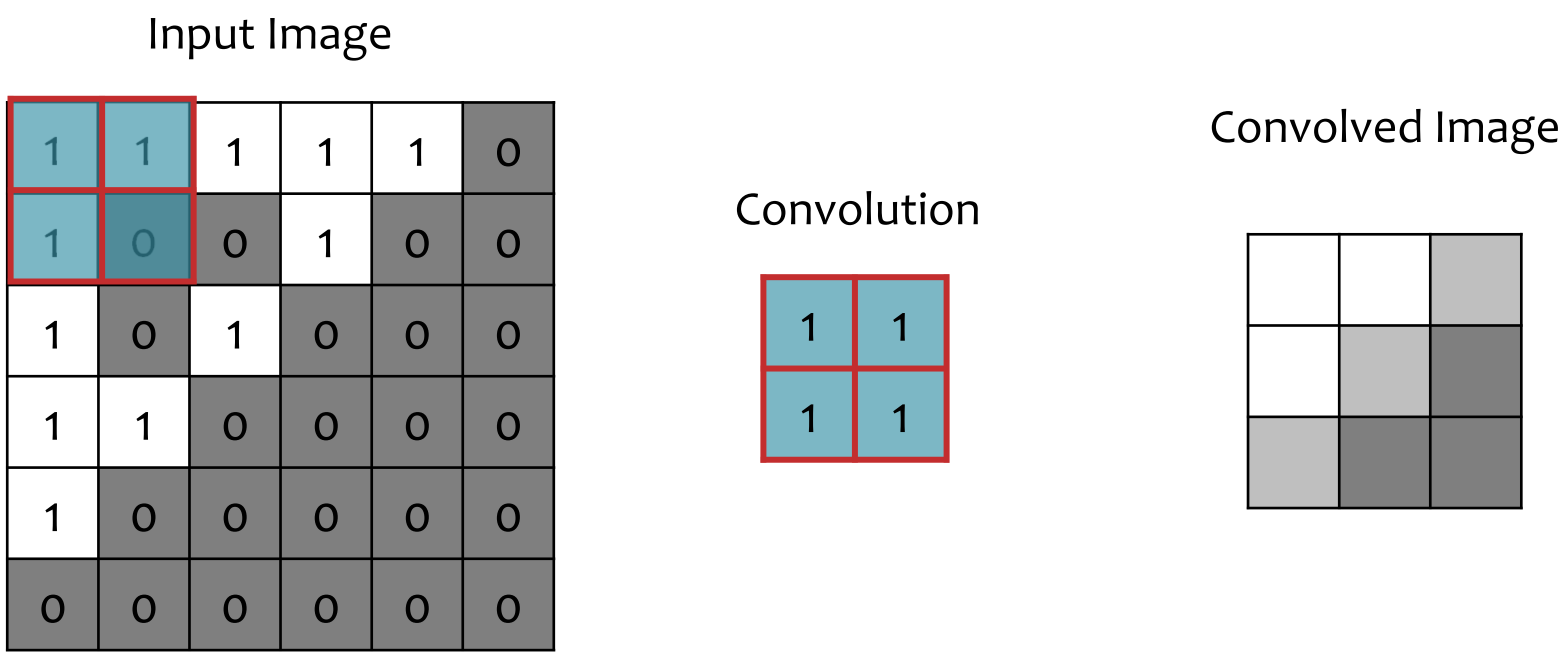
$$y_{22} = \alpha_{11}x_{22} + \alpha_{12}x_{23} + \alpha_{21}x_{32} + \alpha_{22}x_{33} + \alpha_0$$

Slide adapted from William Cohen

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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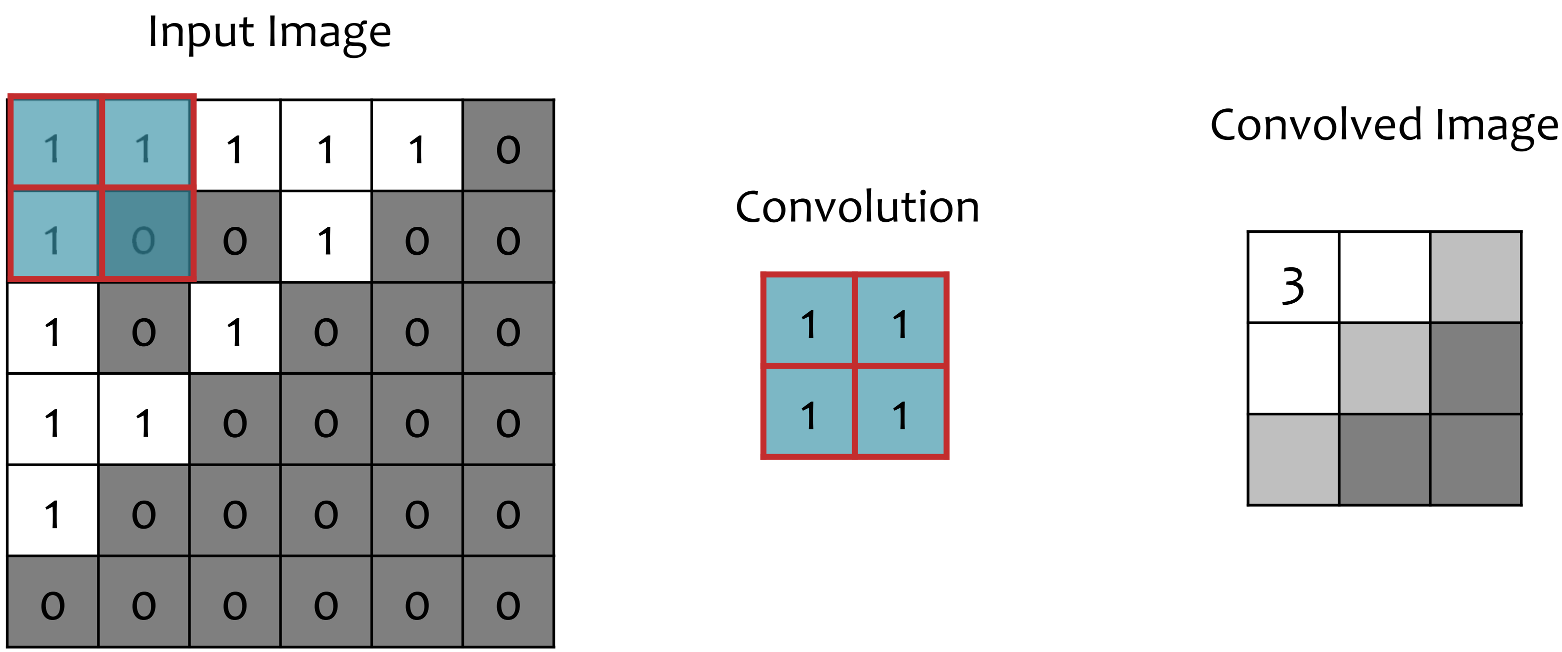

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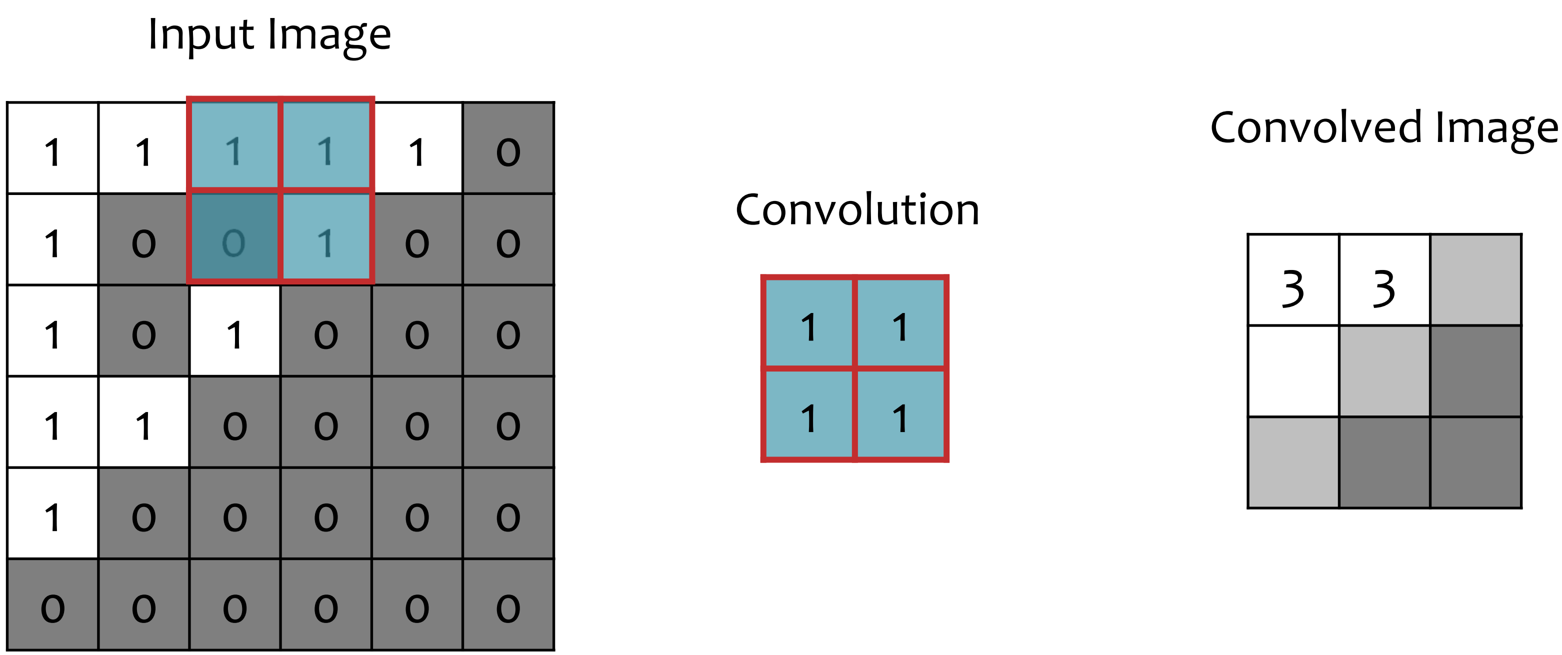

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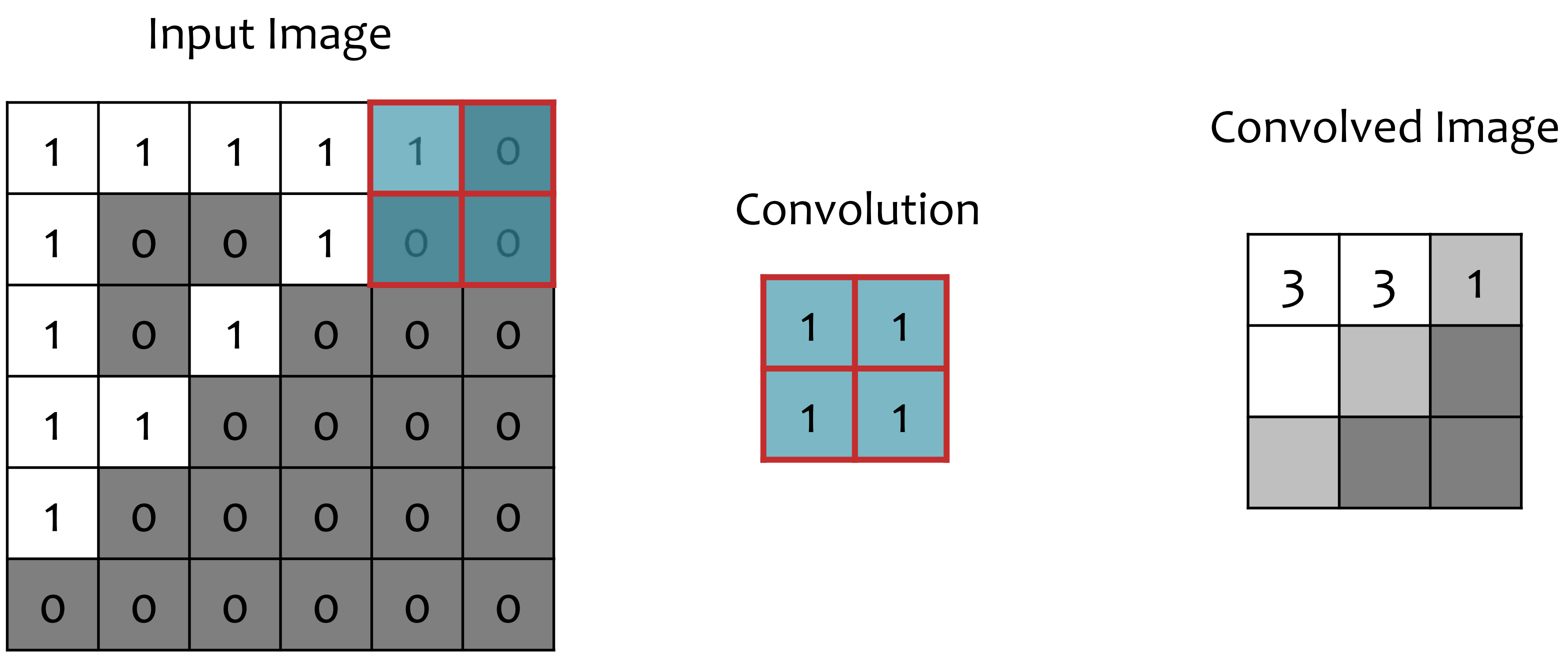

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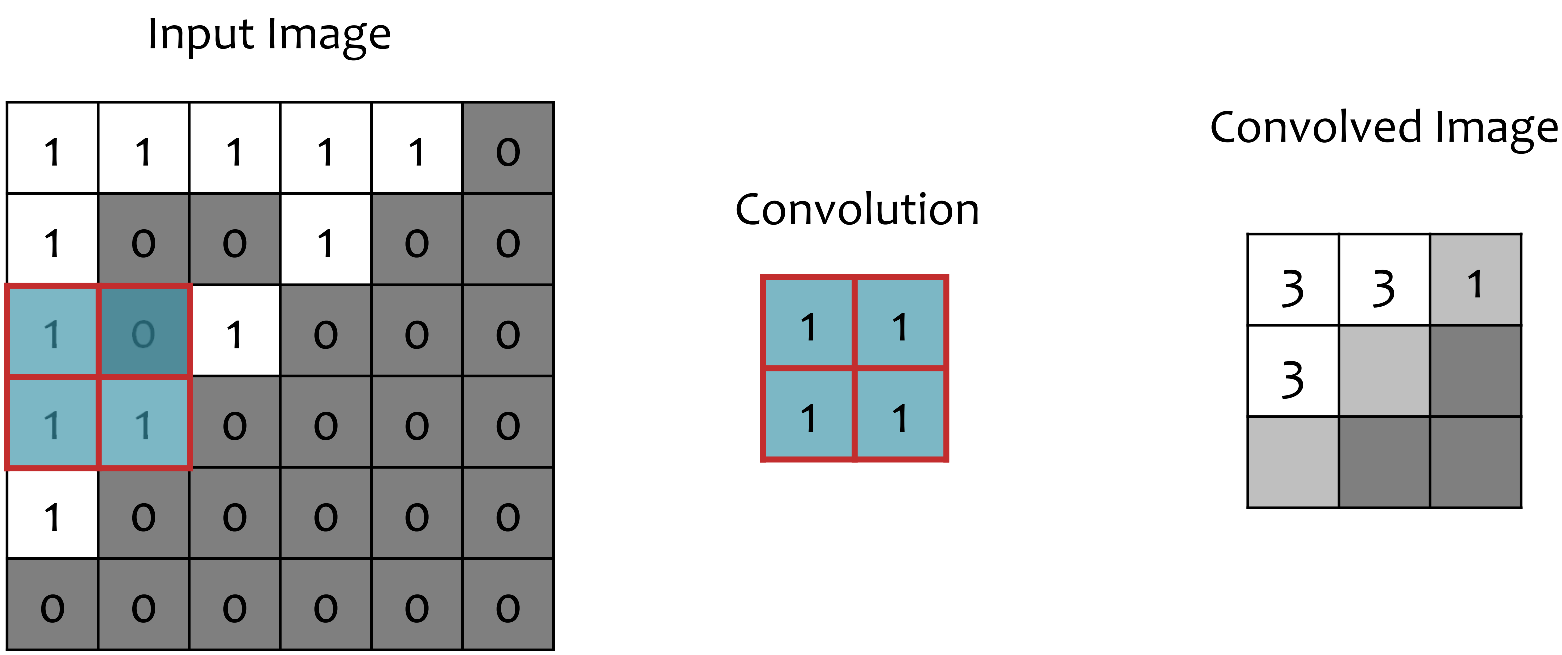

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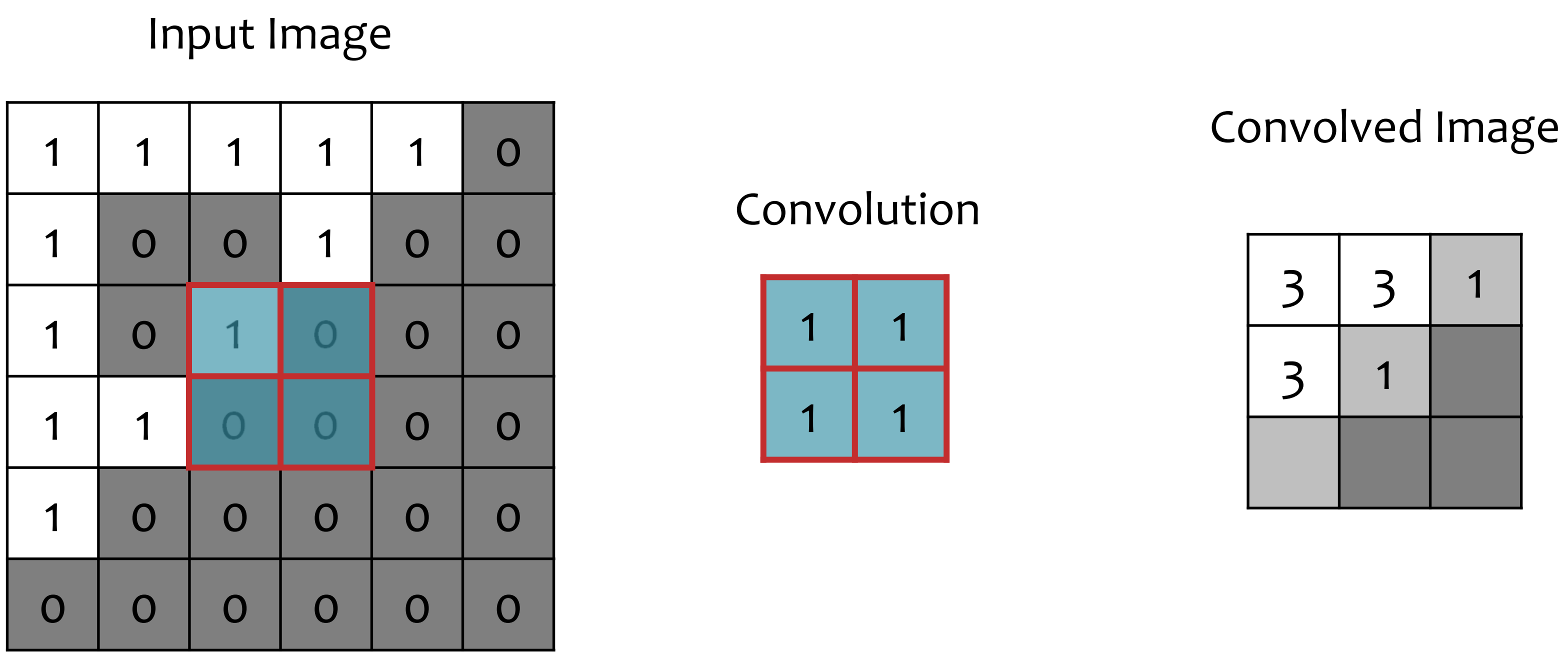

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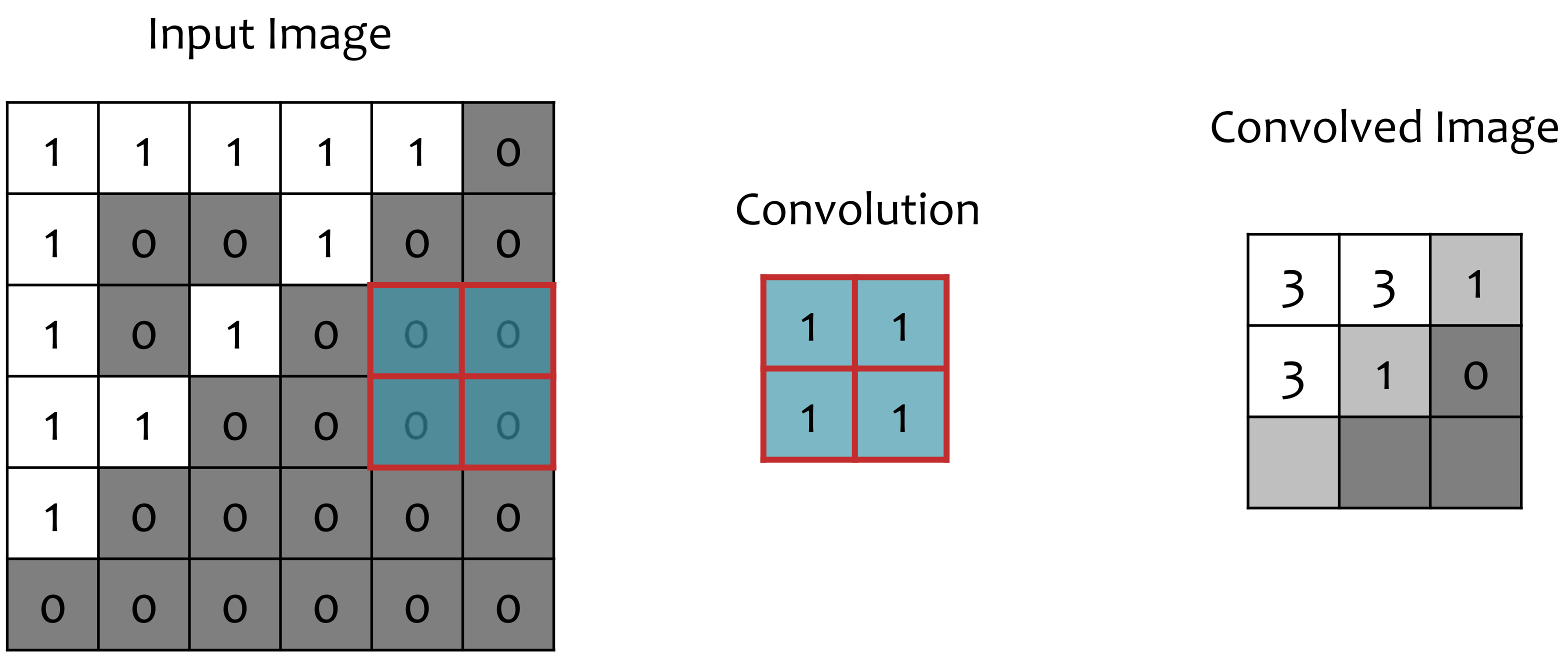

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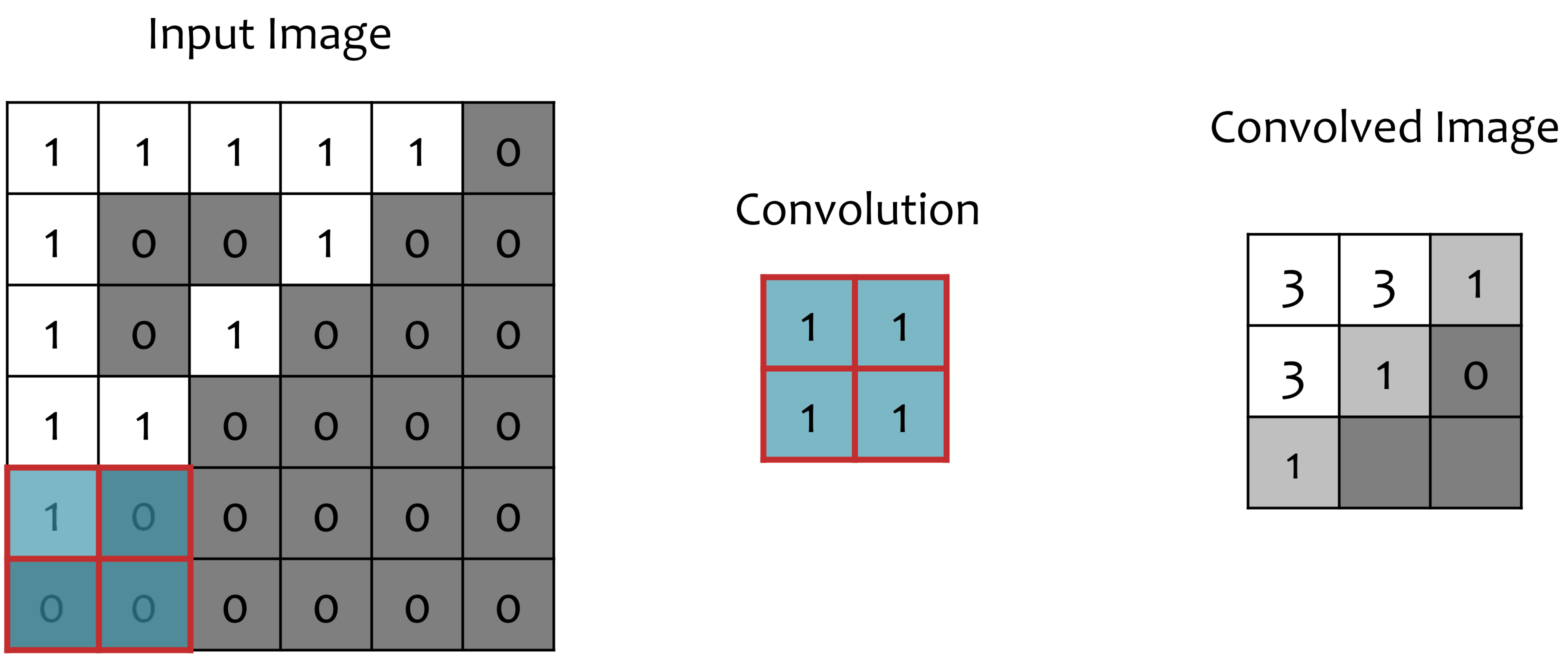

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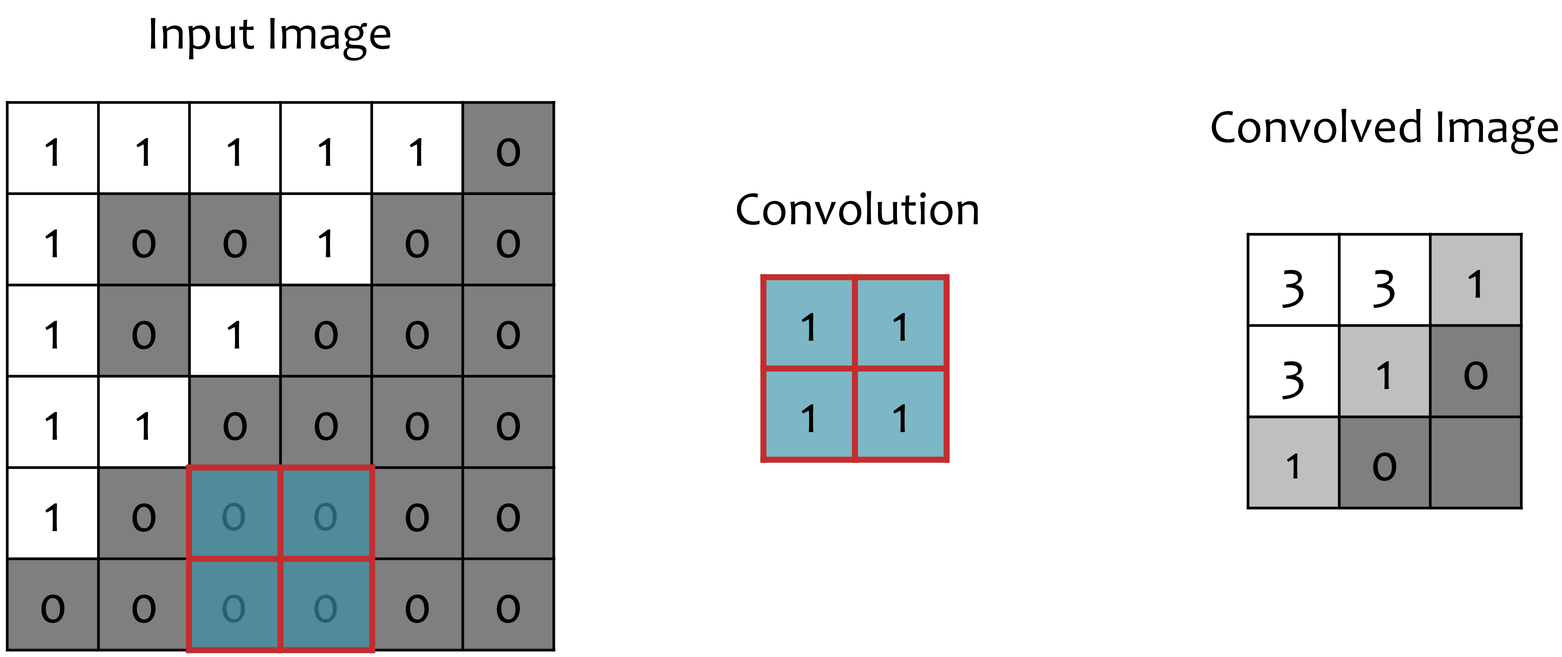

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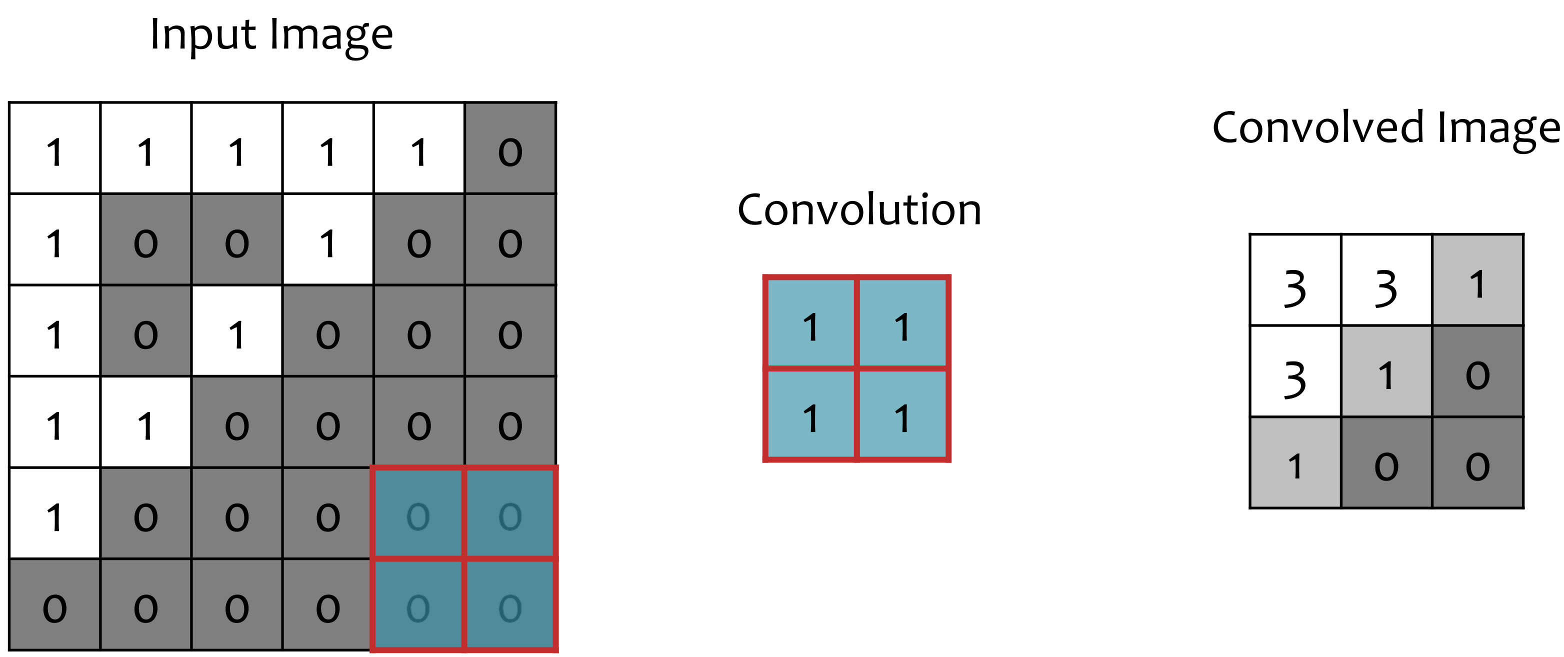

CONVOLUTIONAL NEURAL NETS

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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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

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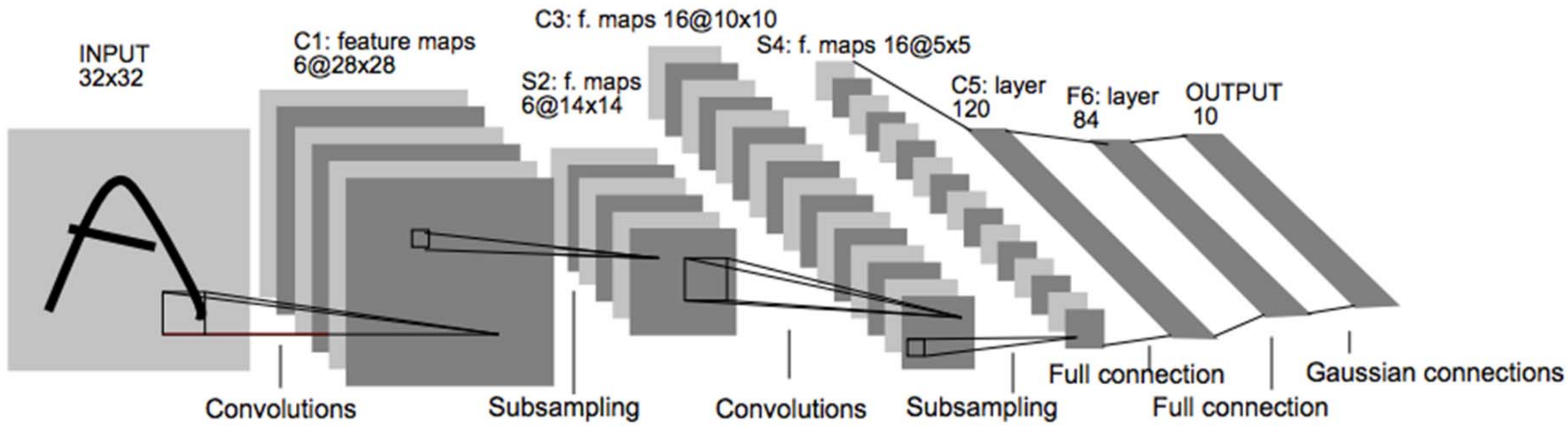


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

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

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

Max-pooling

$x_{i,j}$	$x_{i,j+1}$
$x_{i+1,j}$	$x_{i+1,j+1}$

Max-Pooled Image

1	1	1
1	1	0
1	0	0

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

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:

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

2. Choose each of t

– Decision functio

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

– 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!

opp site the gradient)

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

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 $i \in \{1, \ldots, N\}$
   - Forward: $y = h_\theta(\vec{x}^{(i)})$, $J_i(\theta) = \ell(y, y^*)$
   - Backward: $\nabla_{\vec{\theta}} J_i(\theta) = \ldots$
   - 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

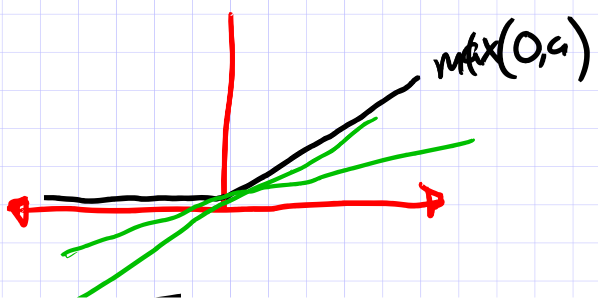
ReLU Layer

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:

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

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

Softmax Layer

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:

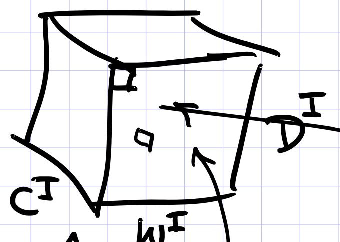
$$\frac{dJ}{dx_j} = \sum_{i=1}^{K} \frac{dJ}{dy_i} \frac{dy_i}{dx_j}$$

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: $X =$



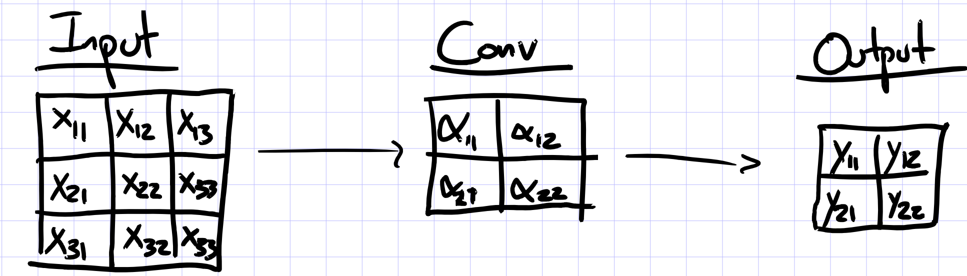
- Stretch out into a long vector: $\hat{x} = [\hat{x}_1, \ldots, \hat{x}_{(C\times H\times W)}]$
- then standard linear layer:

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

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

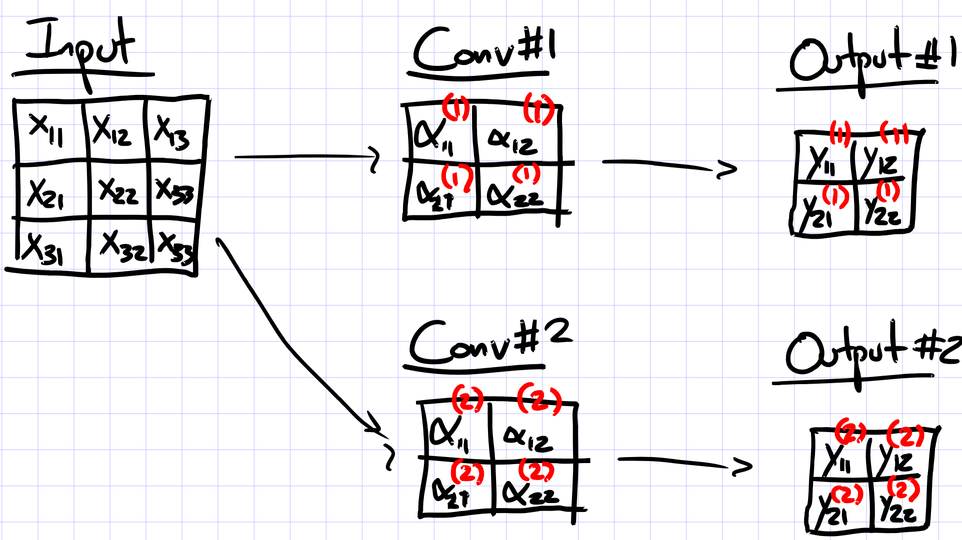
Convolutional Layer

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

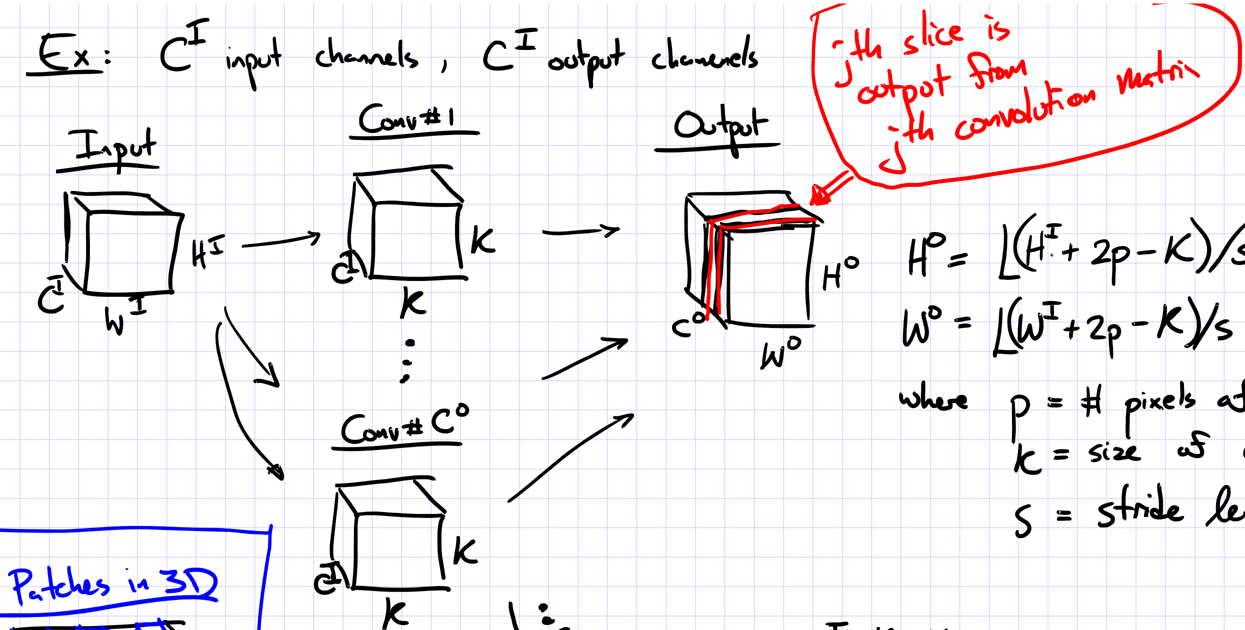


$$y_{11}^{(1)} = \alpha_{11}^{(1)}x_{11} + \alpha_{12}^{(1)}x_{12} + \alpha_{21}^{(1)}x_{21} + \alpha_{22}^{(1)}x_{22} + \alpha_0^{(1)}$$
$$y_{12}^{(1)} = \ldots$$
$$y_{21}^{(1)} = \ldots$$
$$y_{22}^{(1)} = \alpha_{11}^{(1)}x_{22} + \alpha_{12}^{(1)}x_{23} + \alpha_{21}^{(1)}x_{32} + \alpha_{22}^{(1)}x_{33}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

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

Convolutional Layer

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



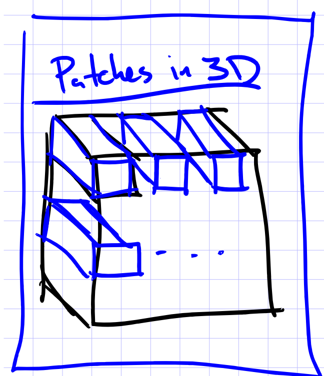
$$H^O = \lfloor (H^I + 2p - K)/s + 1 \rfloor$$

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

where p = # pixels of padding on input

K = size of conv. matrix

s = stride length



Forward:

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

Backward:

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

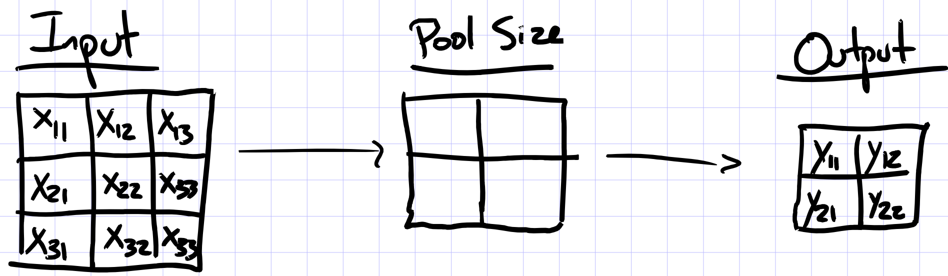
$$\frac{dJ}{d\alpha_{qr}^{(k)}} = \sum_i \sum_j \frac{dJ}{dy_{ij}^{(k)}} \frac{dy_{ij}^{(k)}}{d\alpha_{qr}^{(k)}}$$

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

just some calculus

Max-Pooling Layer

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

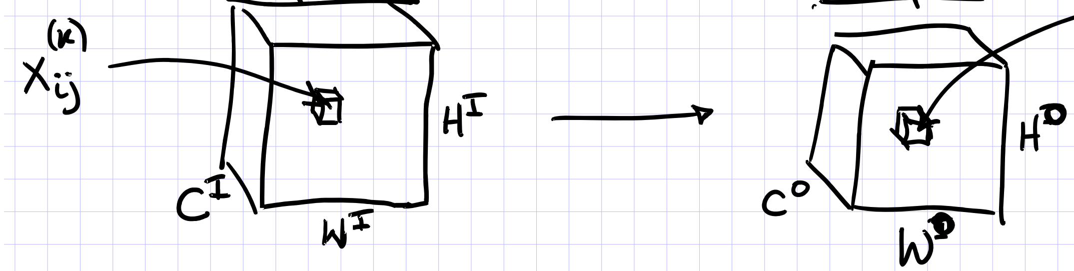


$$y_{11} = \max(x_{11}, x_{12}, x_{21}, x_{22})$$
$$y_{12} = \max(x_{12}, x_{13}, x_{22}, x_{23})$$
$$y_{21} = \max(x_{21}, x_{22}, x_{31}, x_{32})$$
$$y_{22} = \max(x_{22}, x_{23}, x_{32}, x_{33})$$

Max-Pooling Layer

Max-Pooling Layer

Input: Output:



$C^O = C^I$

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

Same hyperparams too.

Forward:

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

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

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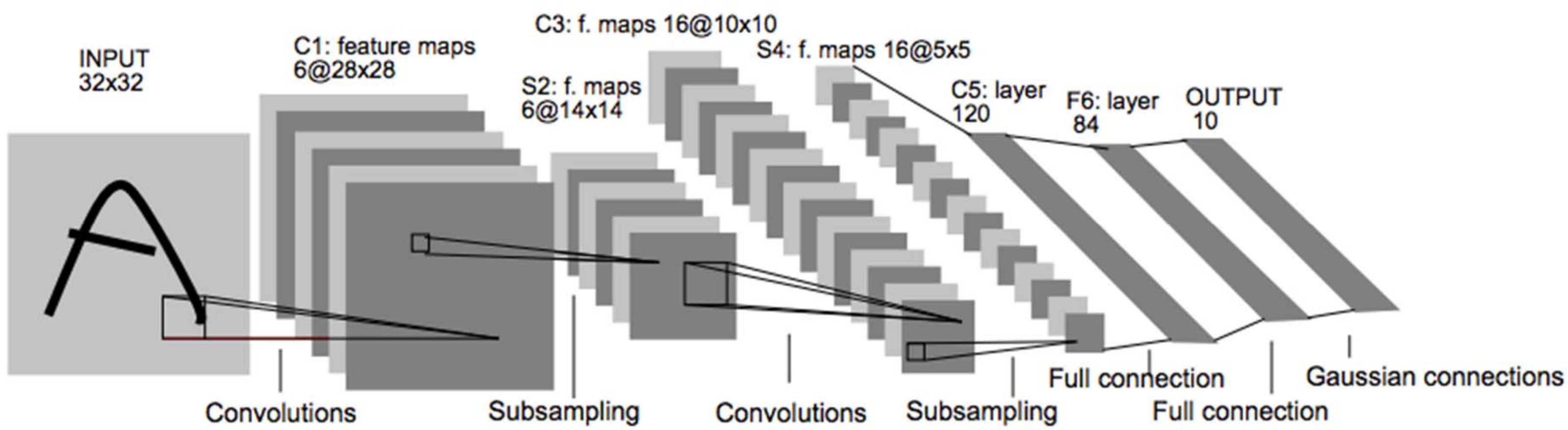


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

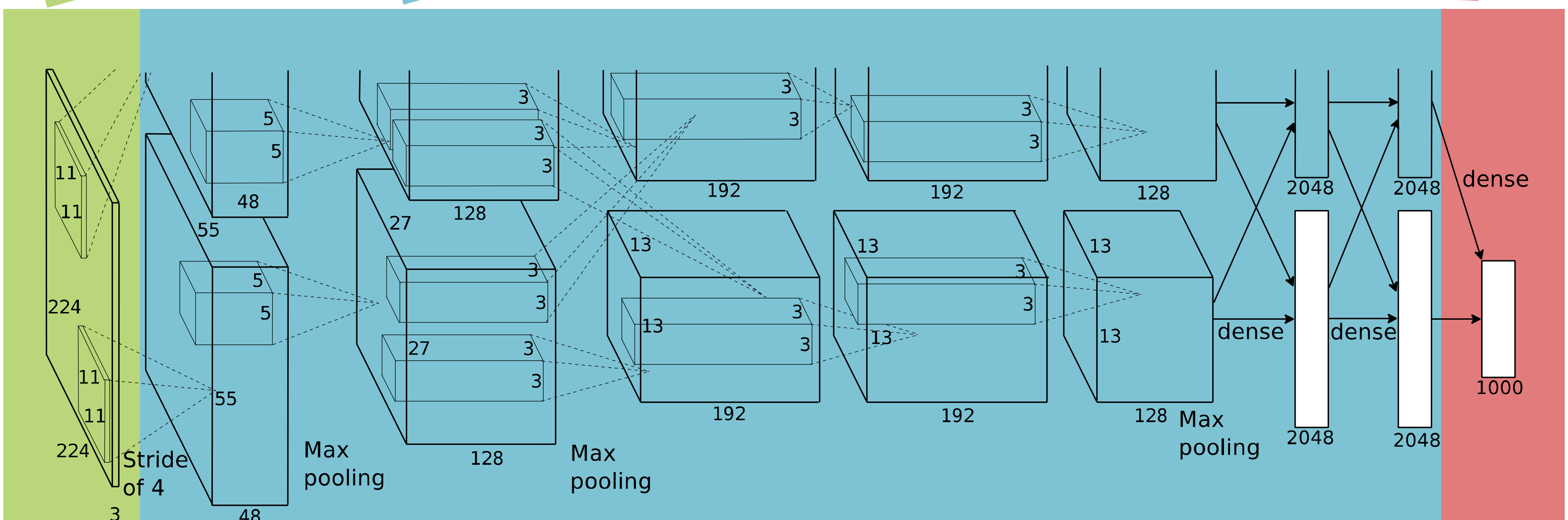
Architecture #2: AlexNet

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

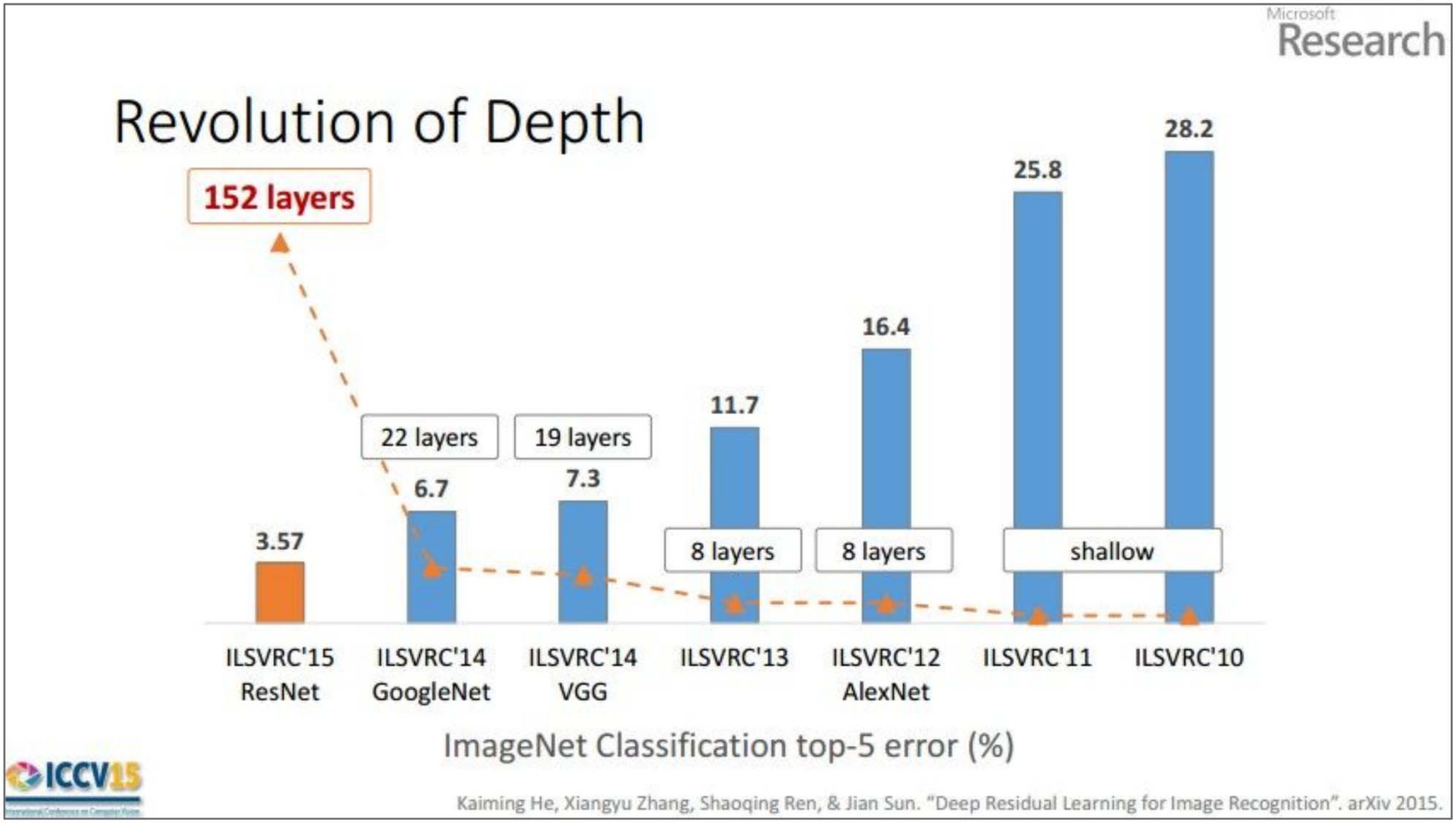
Input image (pixels)

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

1000-way softmax



CNNs for Image Recognition

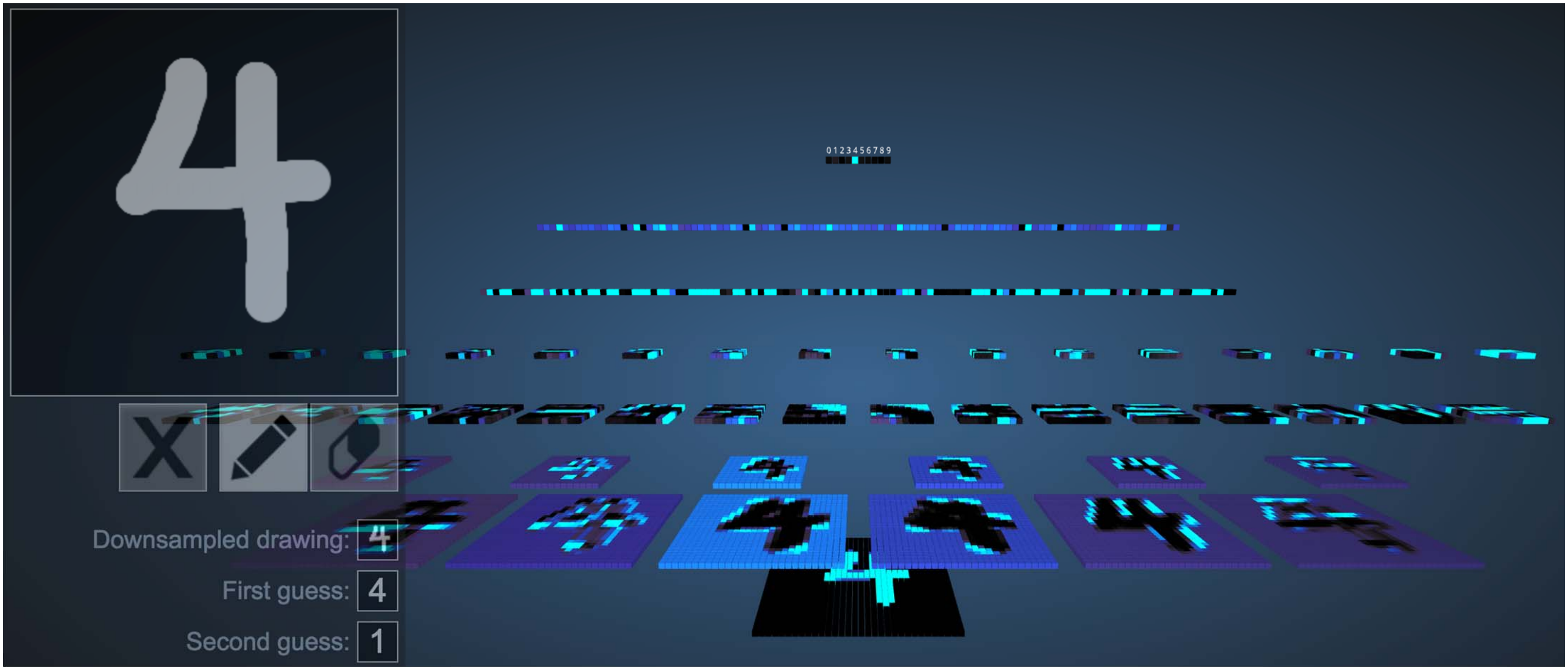


Slide from Kaiming He

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

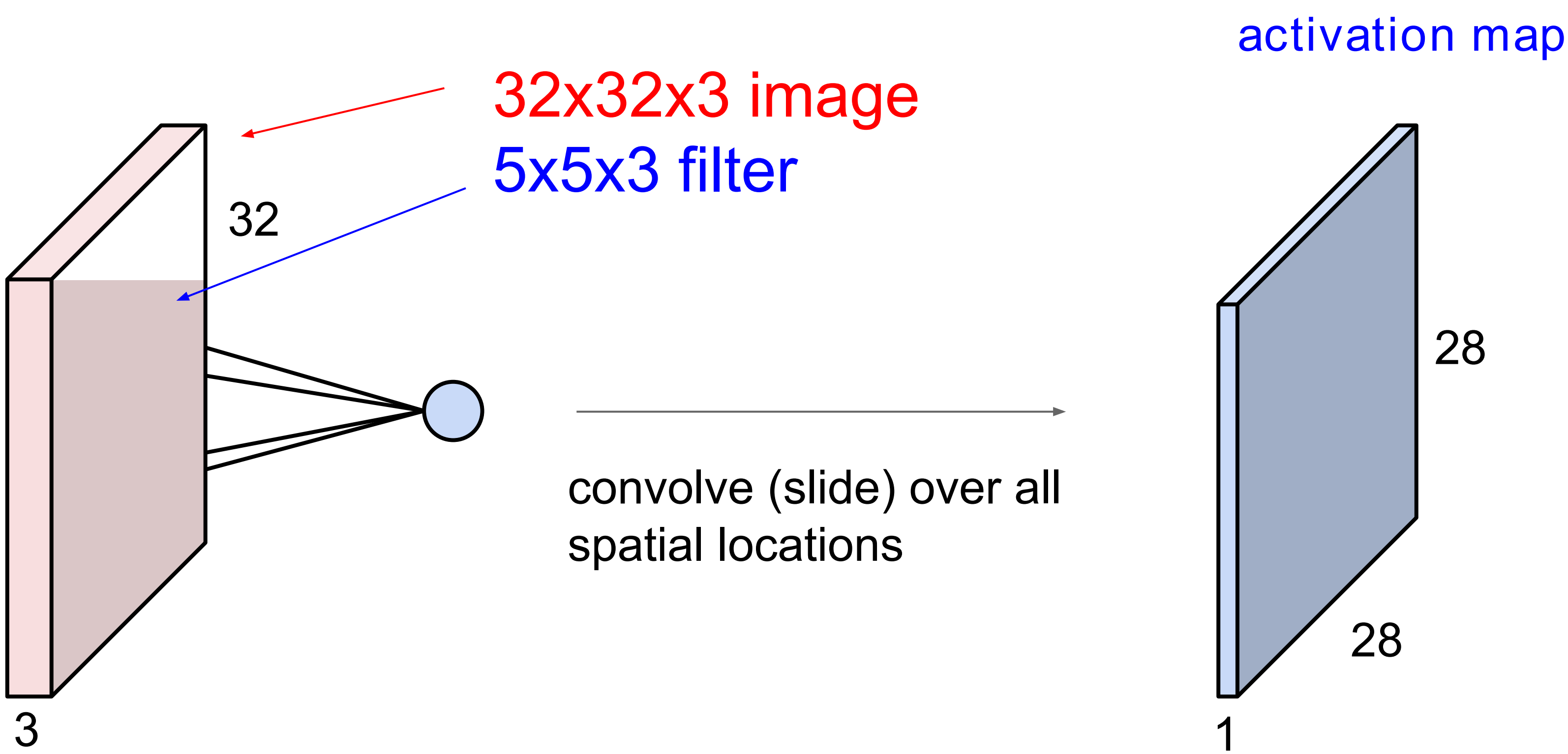


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

Animation of 3D Convolution

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

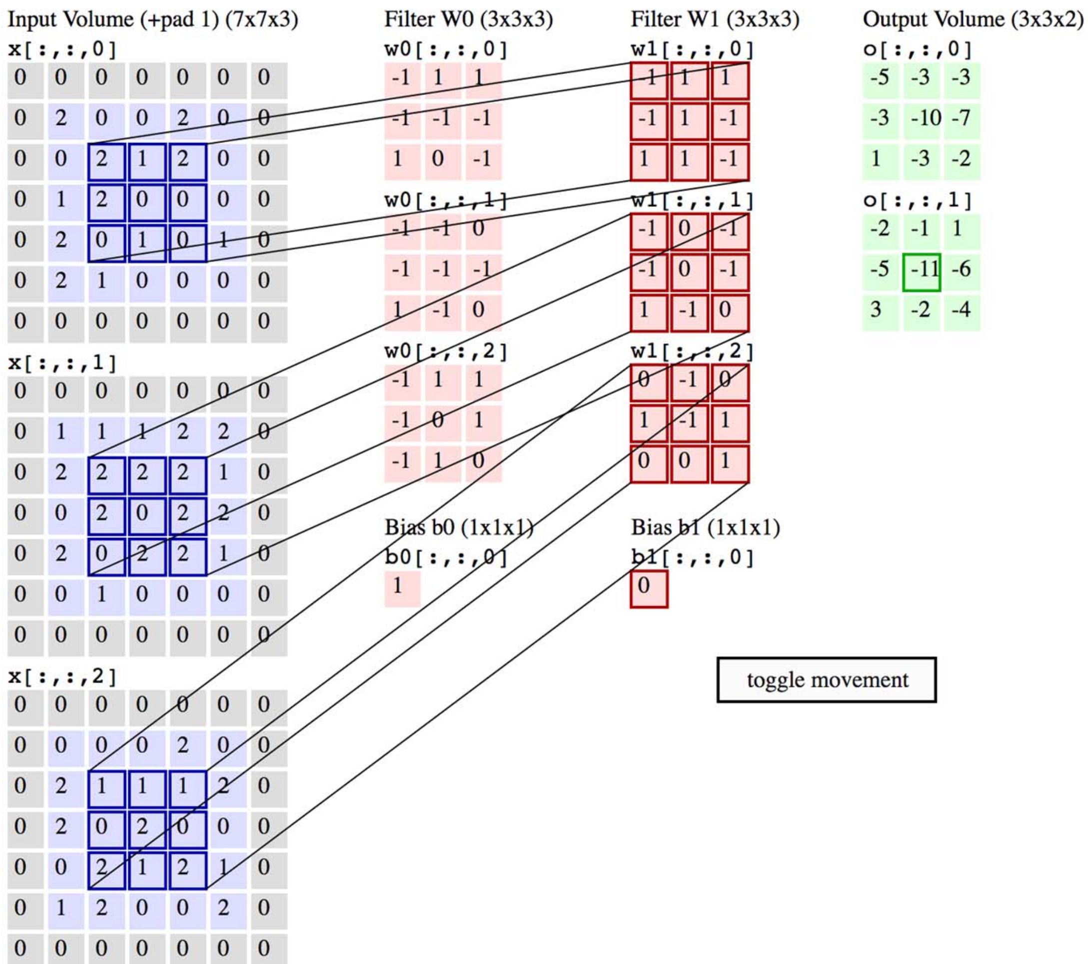


Figure from Fei-Fei Li & Andrej Karpathy & Justin Johnson (CS231N)

MNIST Digit Recognition with CNNs (in your browser)

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

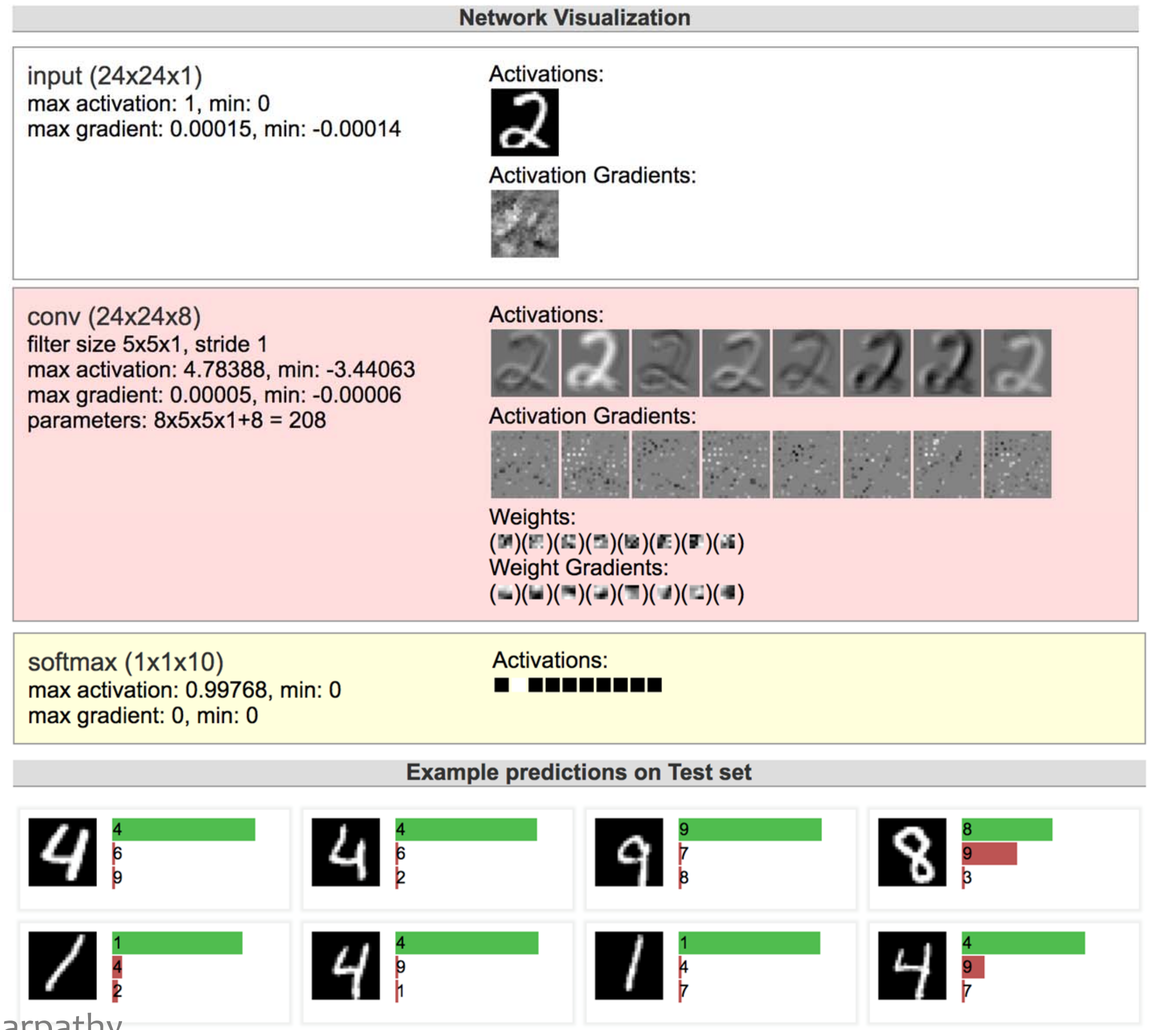


Figure from Andrej Karpathy

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

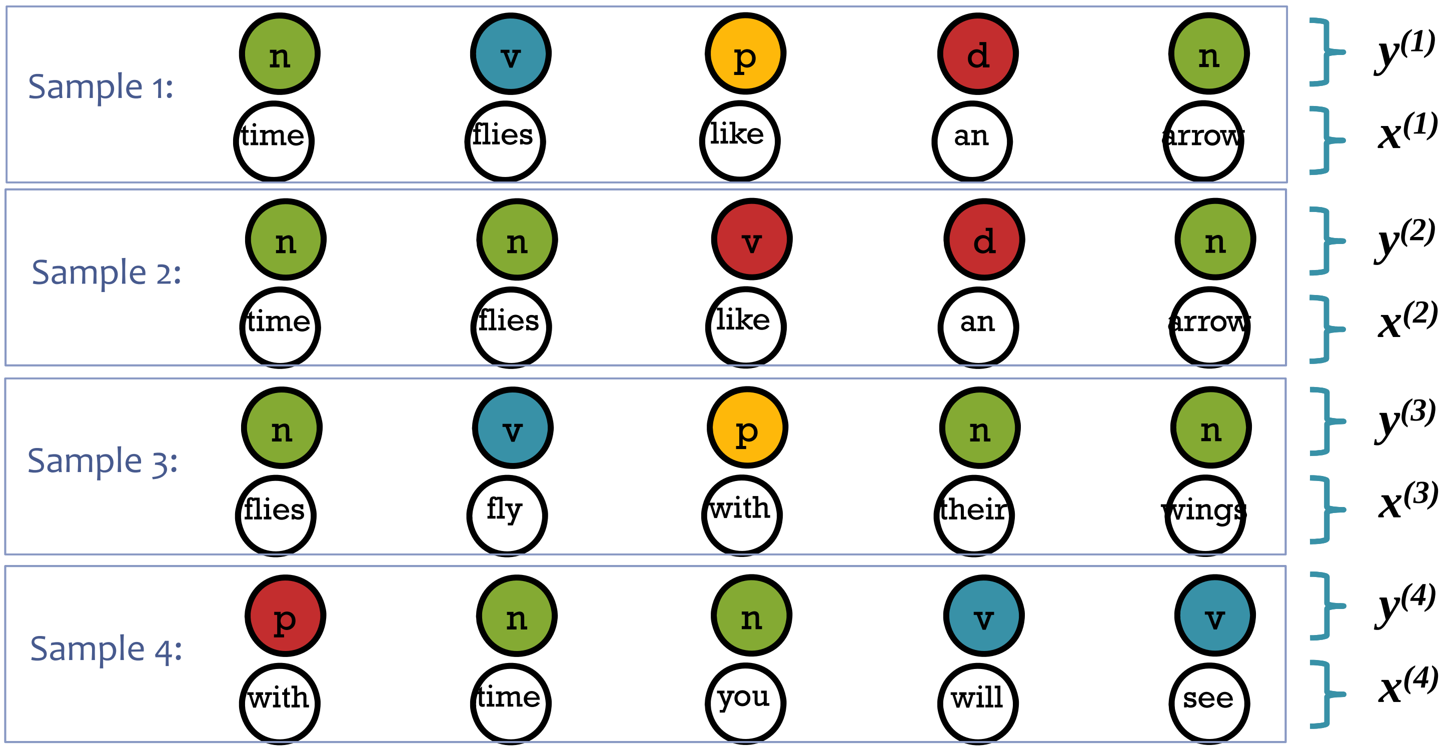
Other Resources:

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

RECURRENT NEURAL NETWORKS

Dataset for Supervised Part-of-Speech (POS) Tagging

Data: $\mathcal{D} = \{\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)}\}_{n=1}^{N}$



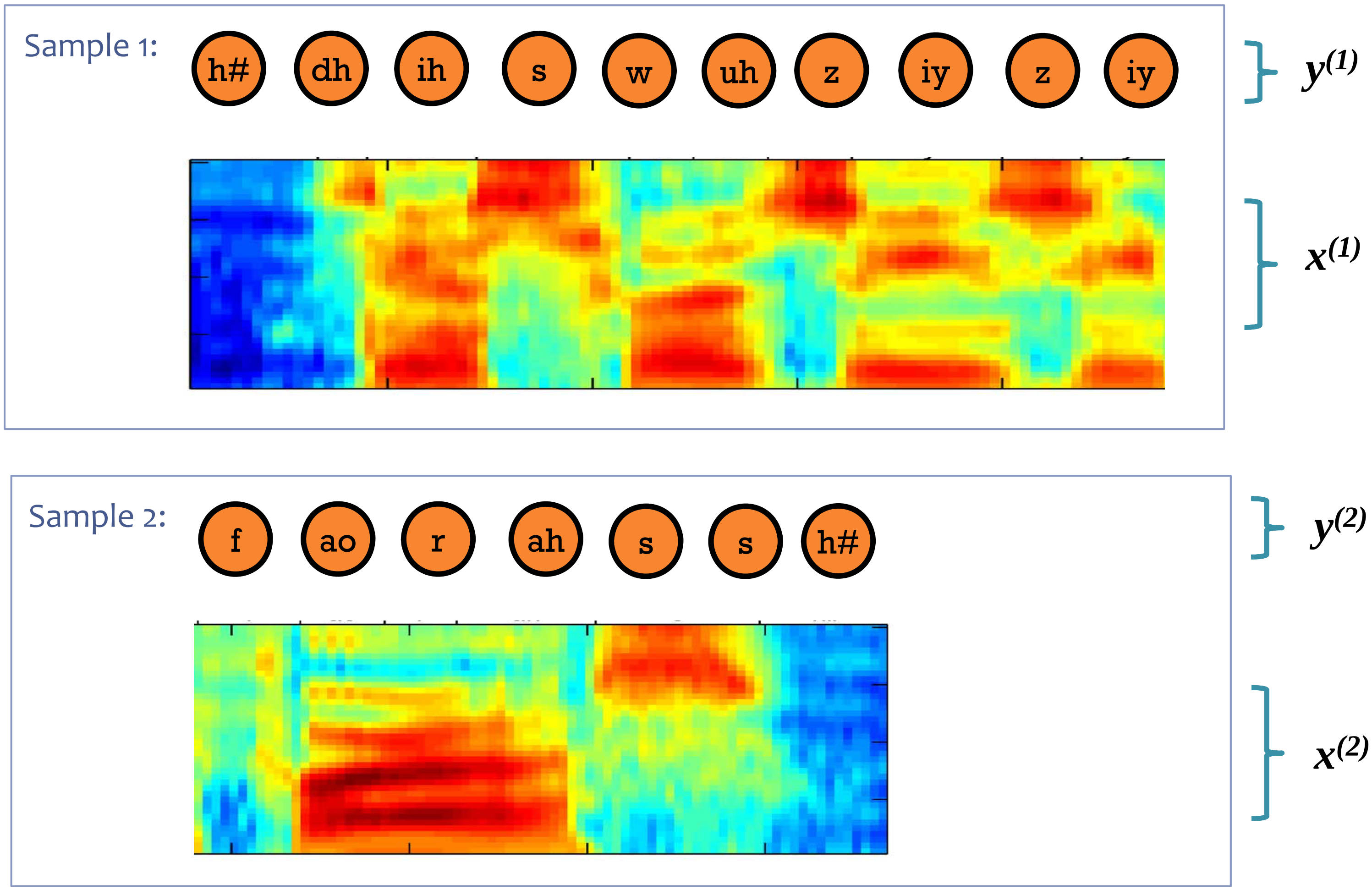
Dataset for Supervised Handwriting Recognition

Data: $\mathcal{D} = \{\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)}\}_{n=1}^{N}$

Figures from (Chatzis & Demiris, 2013)

Dataset for Supervised Phoneme (Speech) Recognition

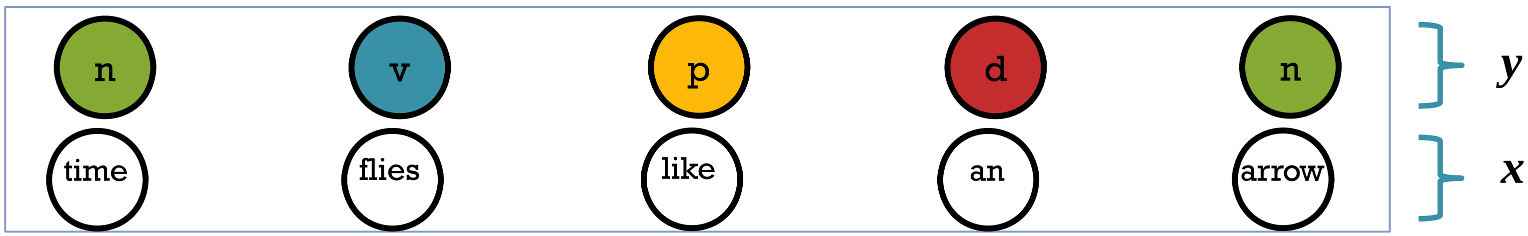
Data: $\mathcal{D} = \{\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)}\}_{n=1}^{N}$



Figures from (Jansen & Niyogi, 2013)

Time Series Data

Question 1: How could we apply the neural networks we've seen so far (which expect **fixed size input/output**) to a prediction task with **variable length input/output**?



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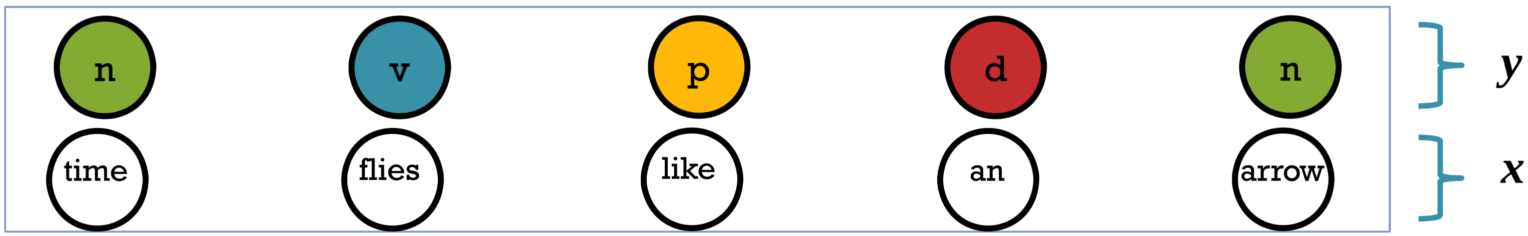
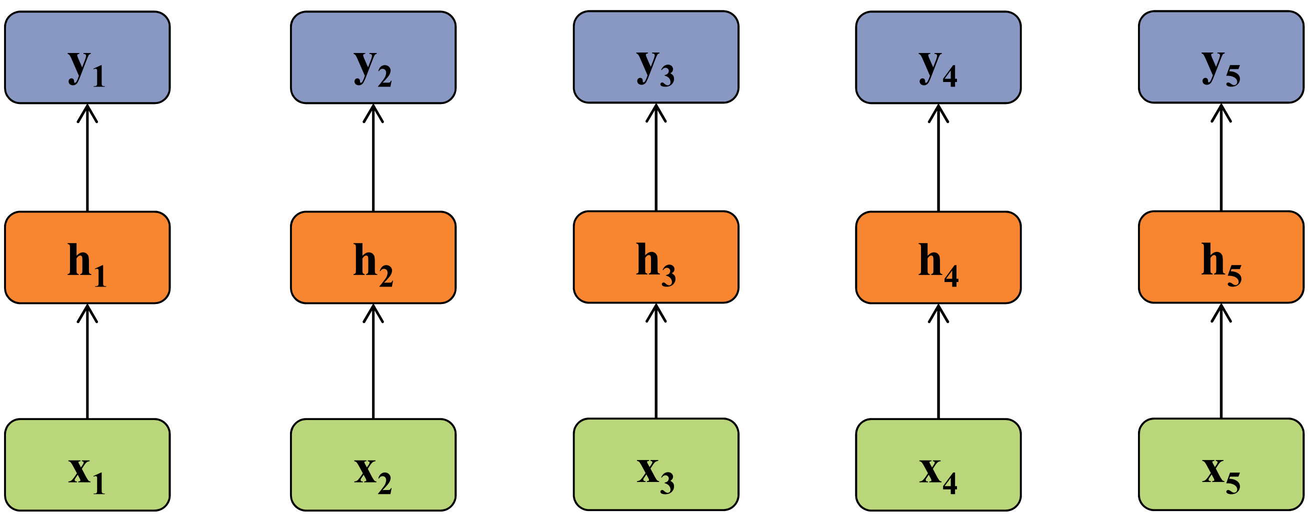
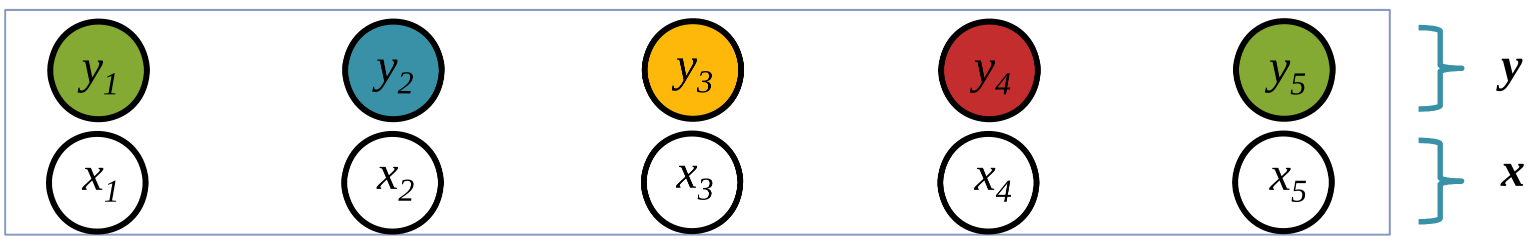




Time Series Data

Question 2: How could we incorporate context (e.g. words to the left/right, or tags to the left/right) into our solution?



Multiple Choice:

Working left-to-right, use features of…

	x_{i-1}	x_i	x_{i+1}	y_{i-1}	y_i	y_{i+1}
A	✓					
B				✓		
C	✓			✓		
D	✓			✓	✓	✓
E	✓	✓		✓	✓	✓
F	✓	✓	✓	✓		
G	✓	✓	✓	✓	✓	
H	✓	✓	✓	✓	✓	✓

Recurrent Neural Networks (RNNs)

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J$

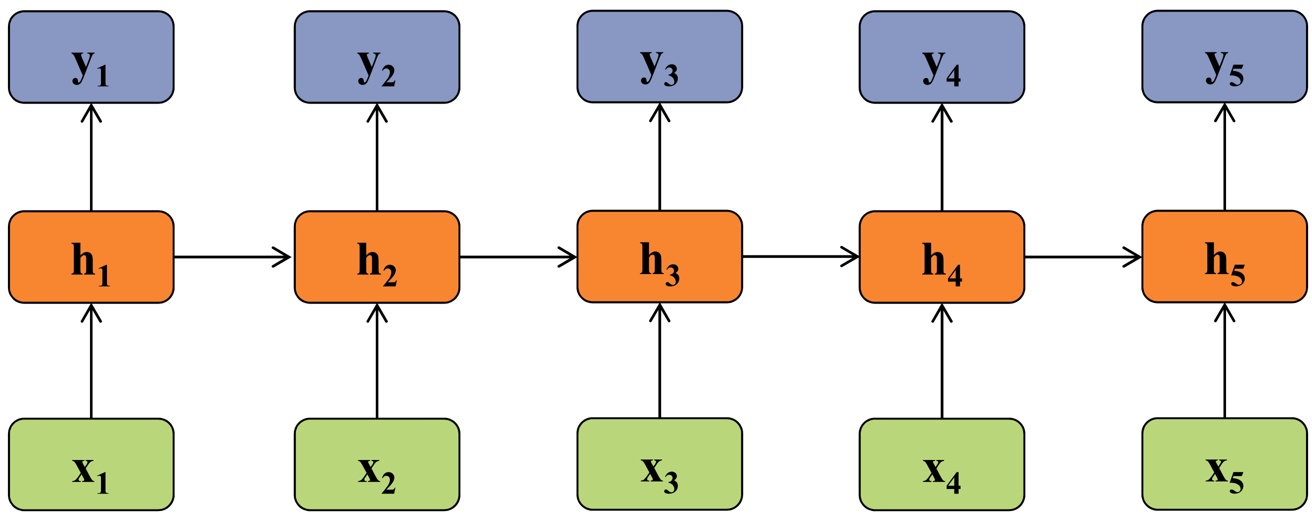
outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$



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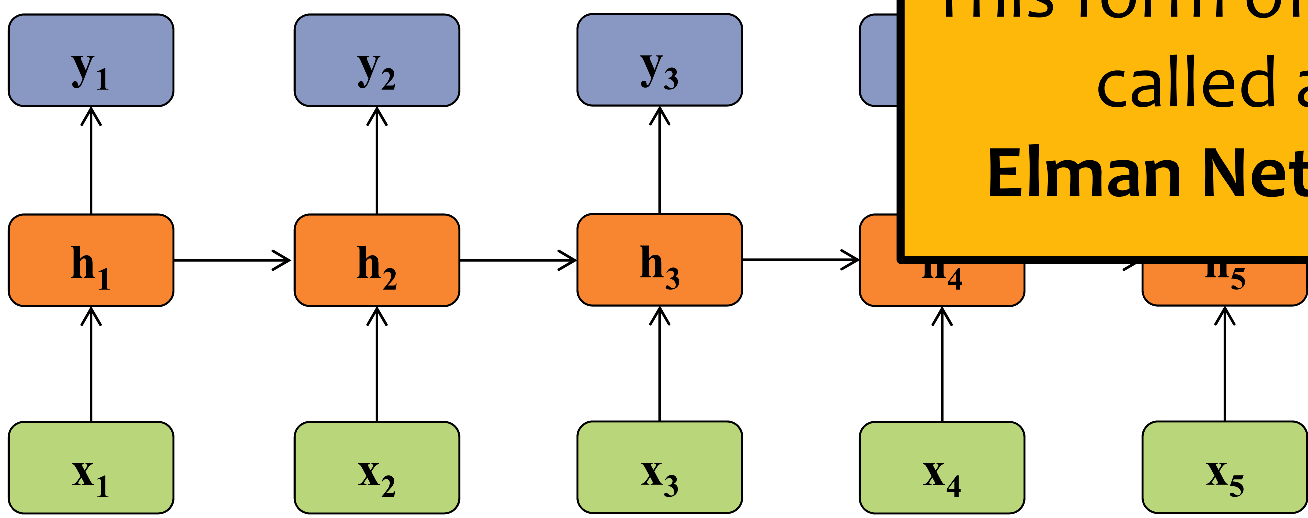
This form of RNN is called an **Elman Network**



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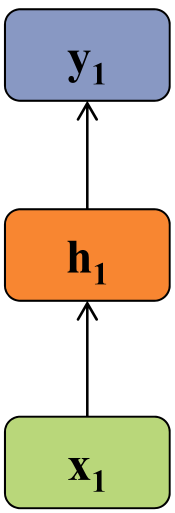

- If T=1, then we have a standard feed-forward **neural net with one hidden layer**
- All of the deep nets from last lecture required **fixed size inputs/outputs**

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)

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

A Recipe for Machine Learning

- Recurrent Neural Networks (RNNs) provide another form of **decision function**
- An RNN is just another differential function

2. Choose each of these:
   - Decision function

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

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

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

- We'll just need a method of computing the gradient efficiently
- Let's use Backpropagation Through Time...

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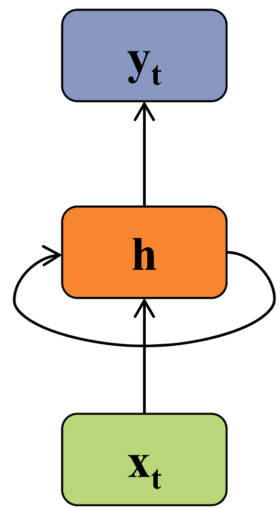

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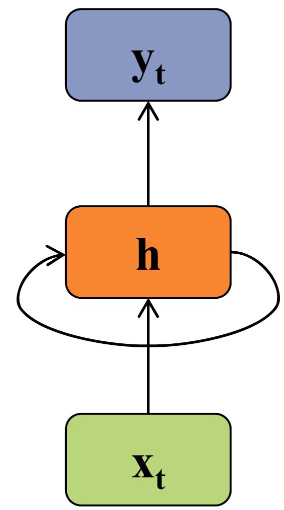
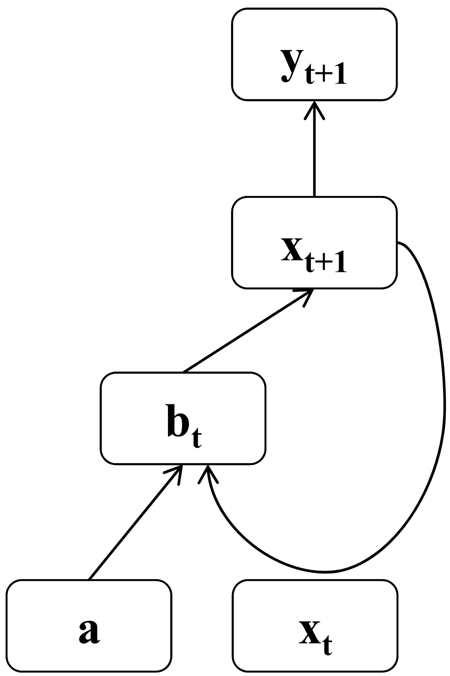
- By unrolling the RNN through time, we can **share parameters** and accommodate **arbitrary length** input/output pairs
- Applications: **time-series data** such as sentences, speech, stock-market, signal data, etc.



Background: Backprop through time

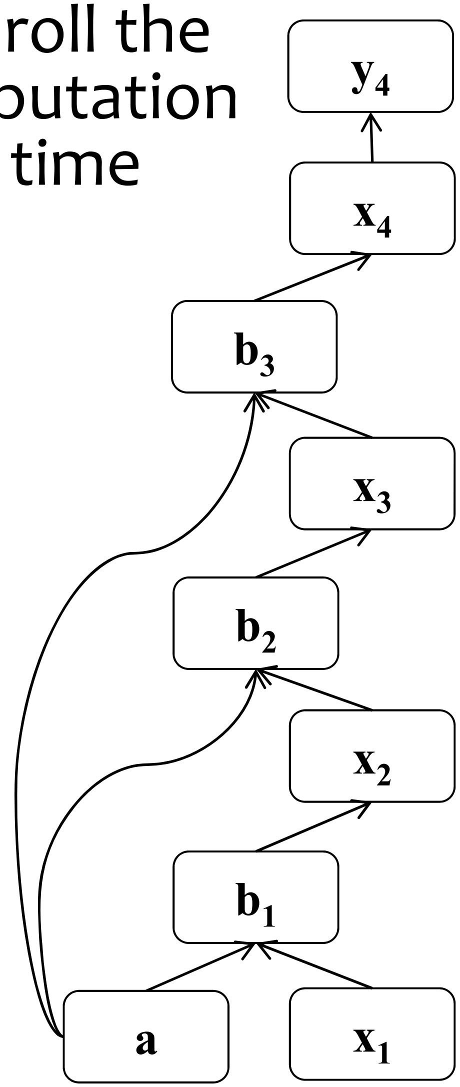
(Robinson & Fallside, 1987)
(Werbos, 1988)
(Mozer, 1995)

Recurrent neural network:



BPTT:

1. Unroll the computation over time



2. Run backprop through the resulting feed-forward network

Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

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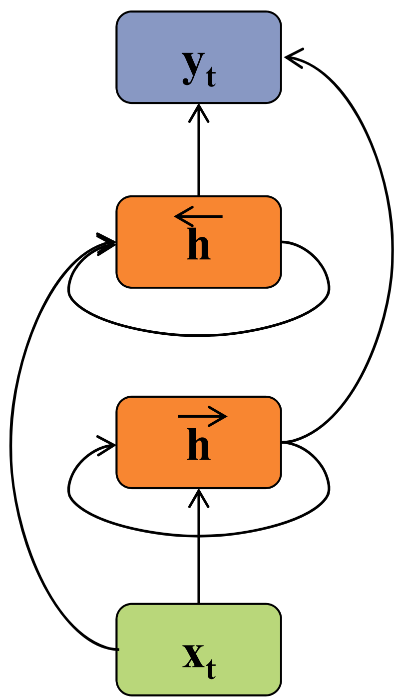
nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

$$\overleftarrow{h}_t = \mathcal{H}\left(W_{x\overleftarrow{h}} x_t + W_{\overleftarrow{h}\overleftarrow{h}} \overleftarrow{h}_{t+1} + b_{\overleftarrow{h}}\right)$$

$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



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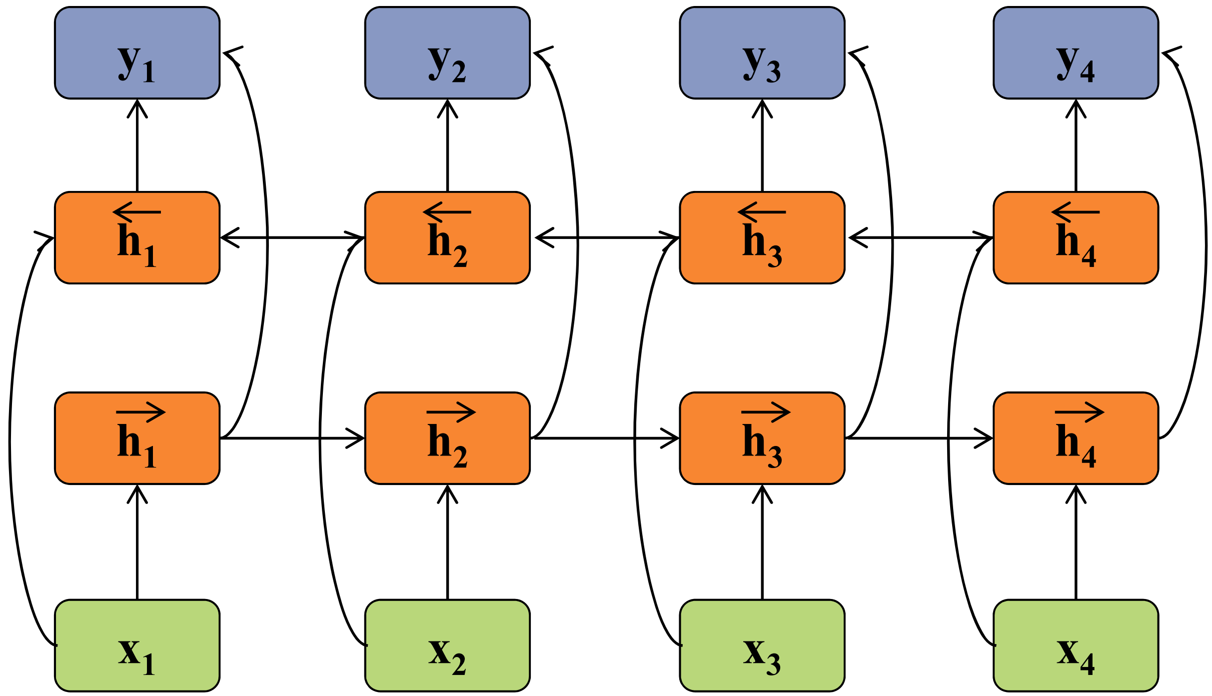

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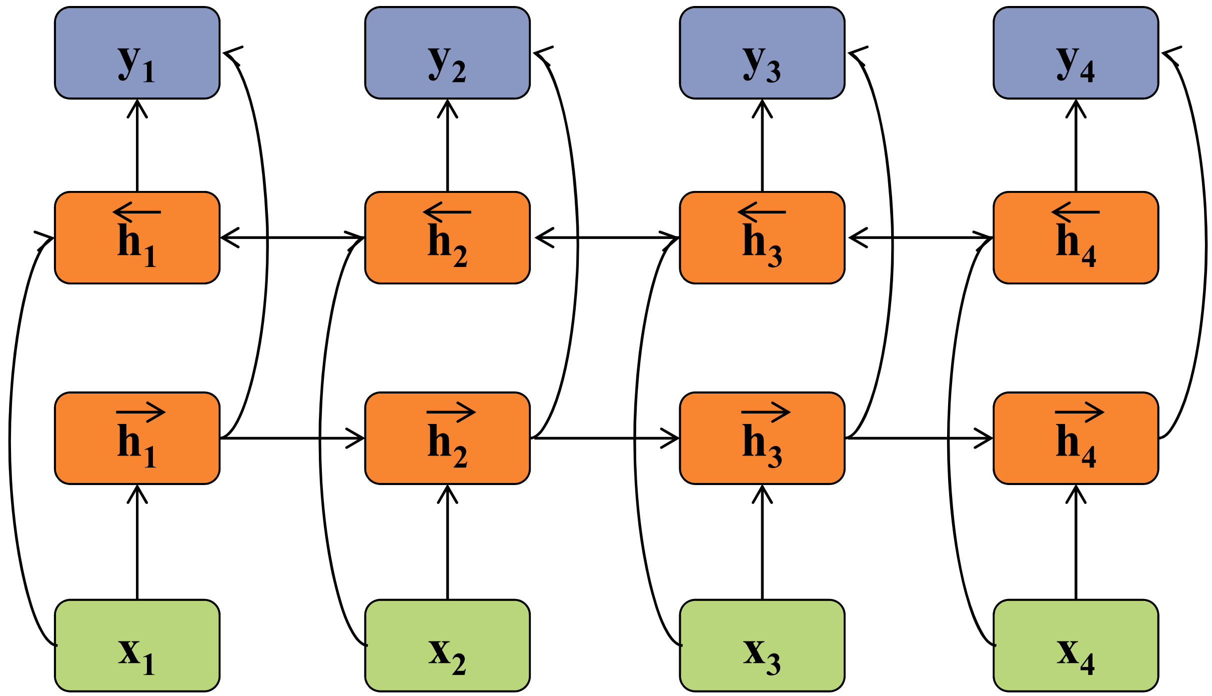

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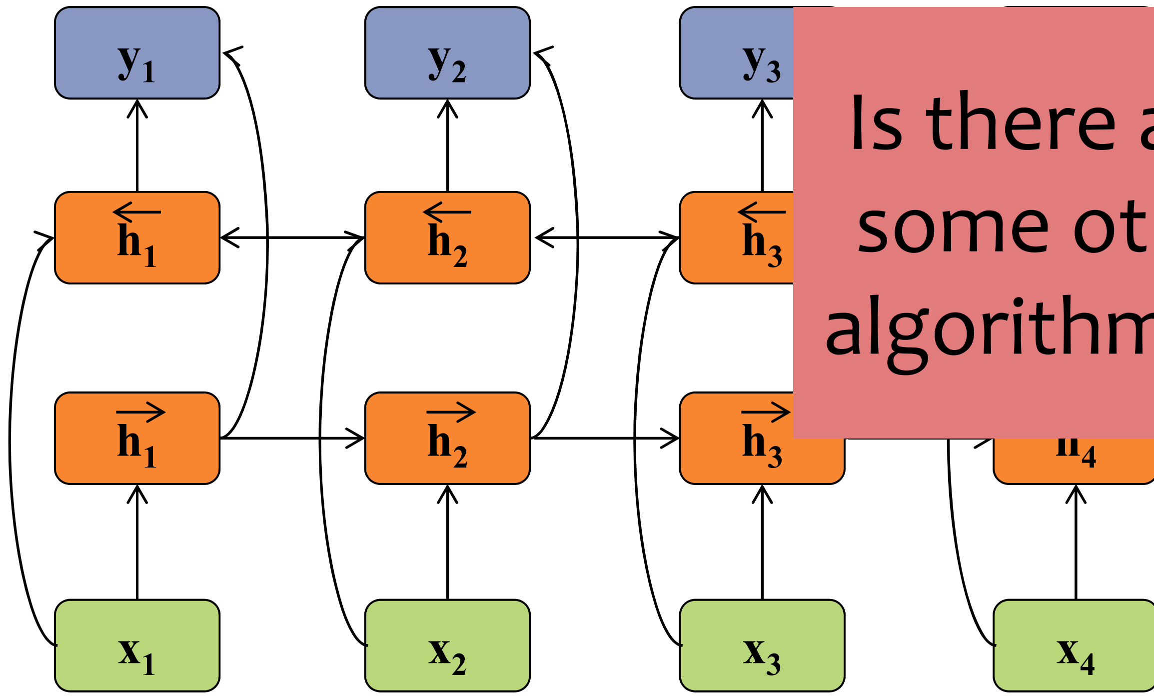

Is there an analogy to some other recursive algorithm(s) we know?

Deep RNNs

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outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$h_t^n = \mathcal{H}\left(W_{h^{n-1}h^n} h_t^{n-1} + W_{h^n h^n} h_{t-1}^n + b_h^n\right)$$

$$y_t = W_{h^N y} h_t^N + b_y$$

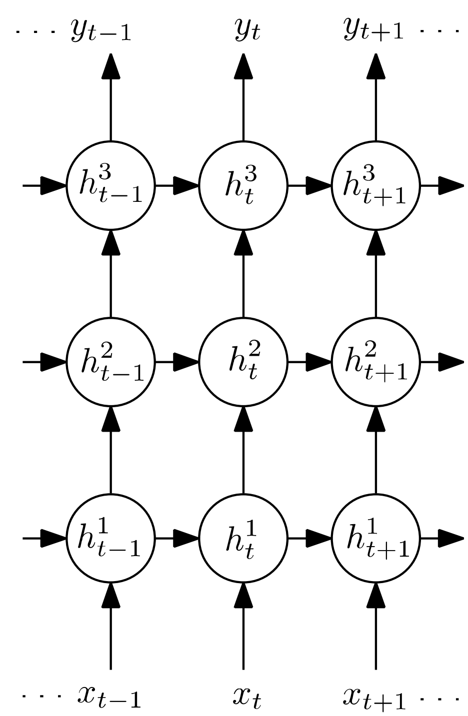

Figure from (Graves et al., 2013)

Deep Bidirectional RNNs

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$$\text{outputs: } \mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$$
$$\text{nonlinearity: } \mathcal{H}$$

- Notice that the upper level hidden units have input from **two previous layers** (i.e. wider input)
- Likewise for the output layer
- What analogy can we draw to DNNs, DBNs, DBMs?

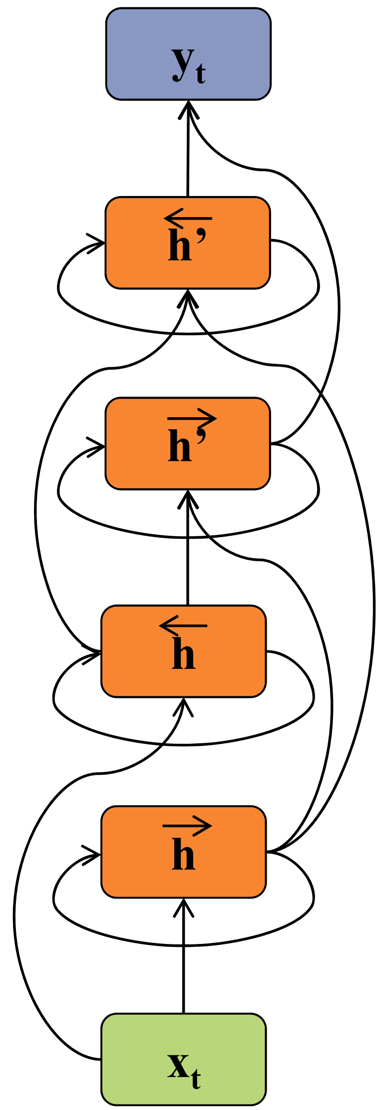
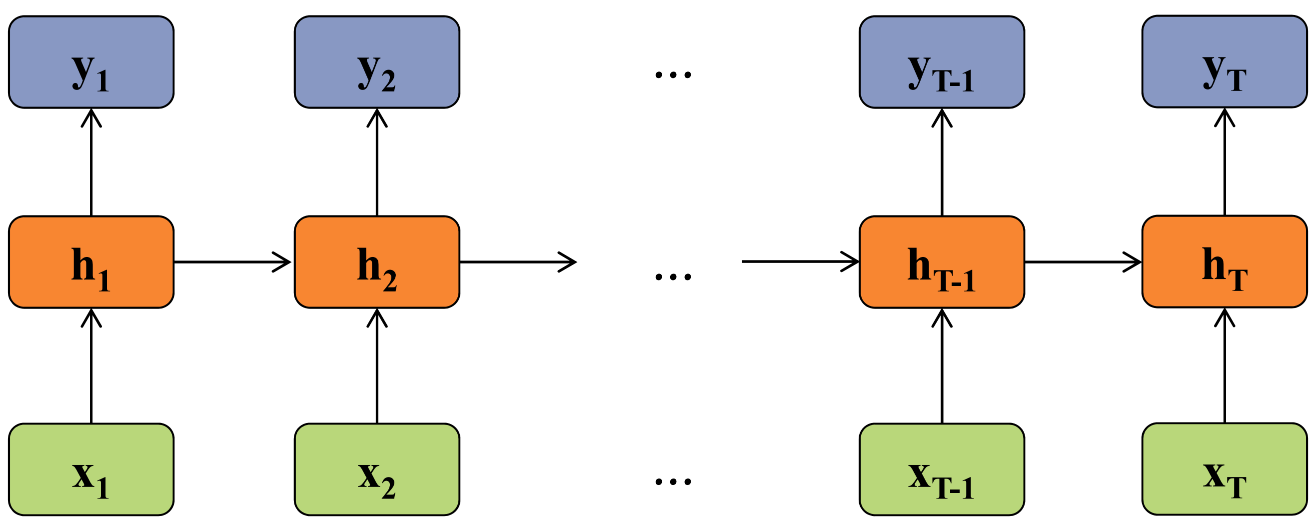


Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)

Motivation:

- Standard RNNs have trouble learning long distance dependencies
- LSTMs combat this issue



Long Short-Term Memory (LSTM)

Motivation:

- Vanishing gradient problem for Standard RNNs
- Figure shows sensitivity (darker = more sensitive) to the input at time t=1

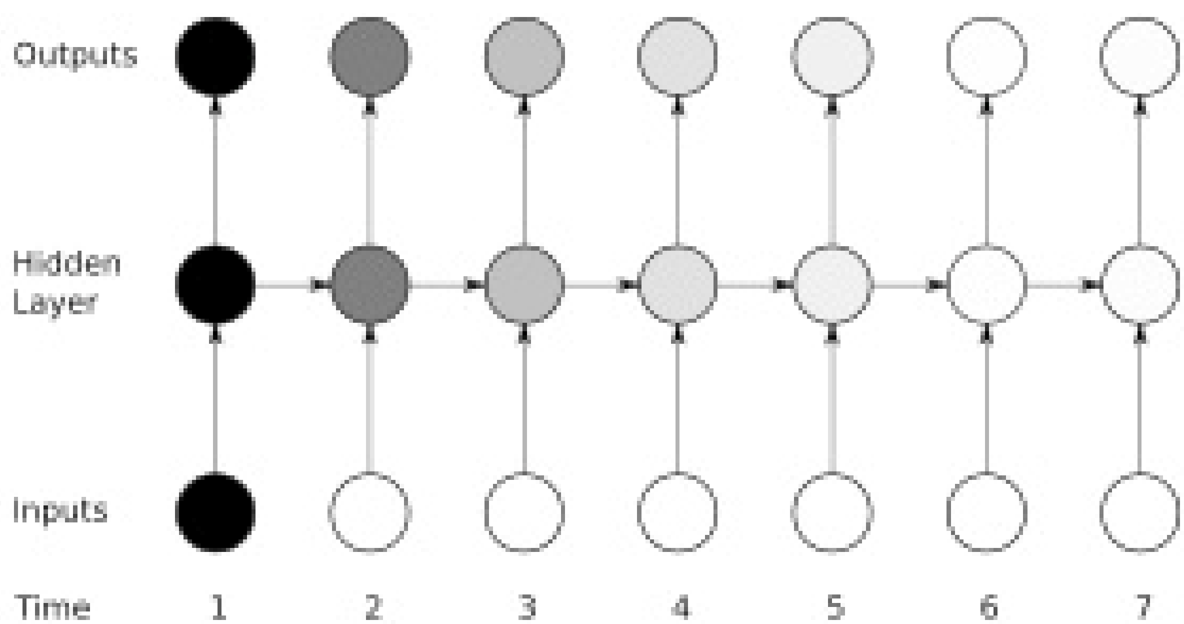


Figure from (Graves, 2012)

Long Short-Term Memory (LSTM)

Motivation:

- LSTM units have a rich internal structure
- The various "gates" determine the propagation of information and can choose to "remember" or "forget" information

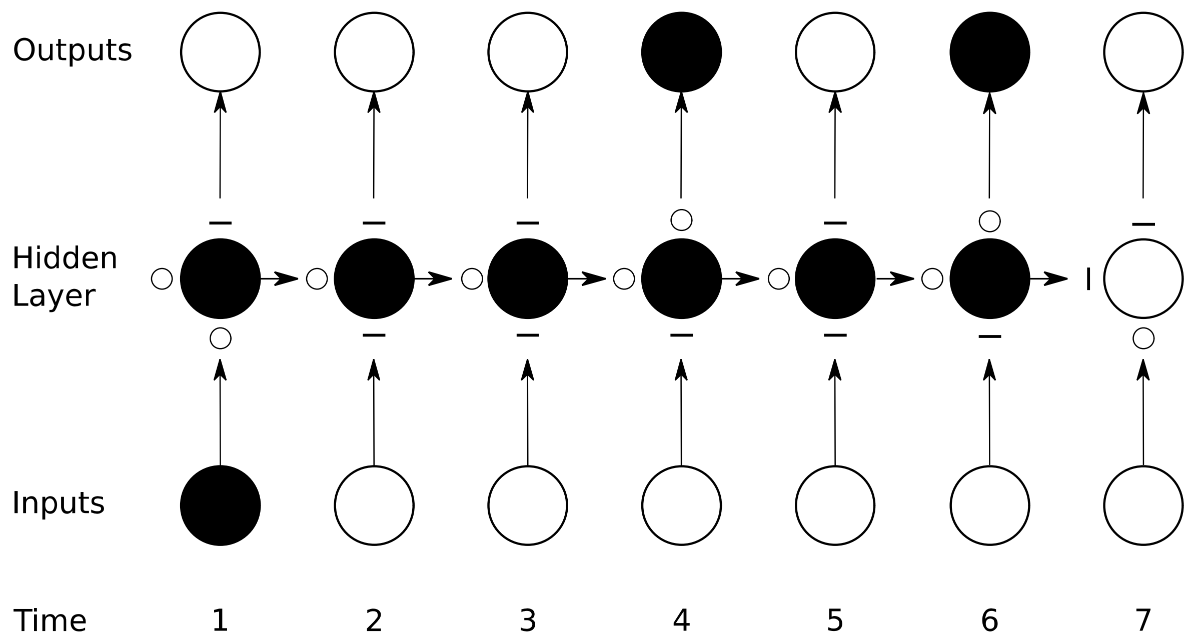


Figure from (Graves, 2012)

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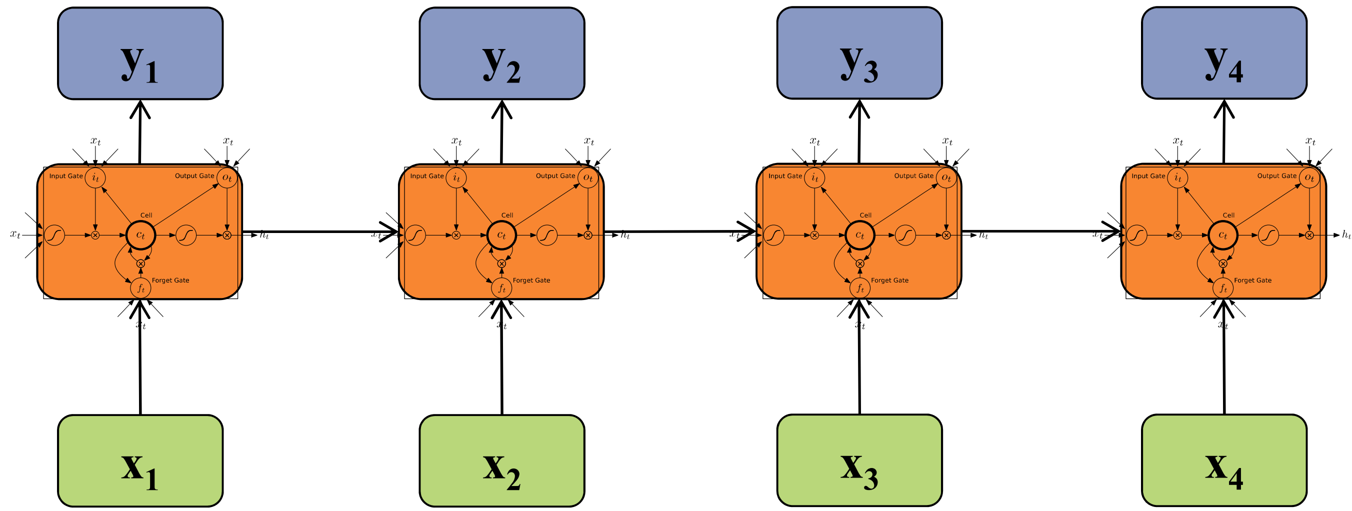
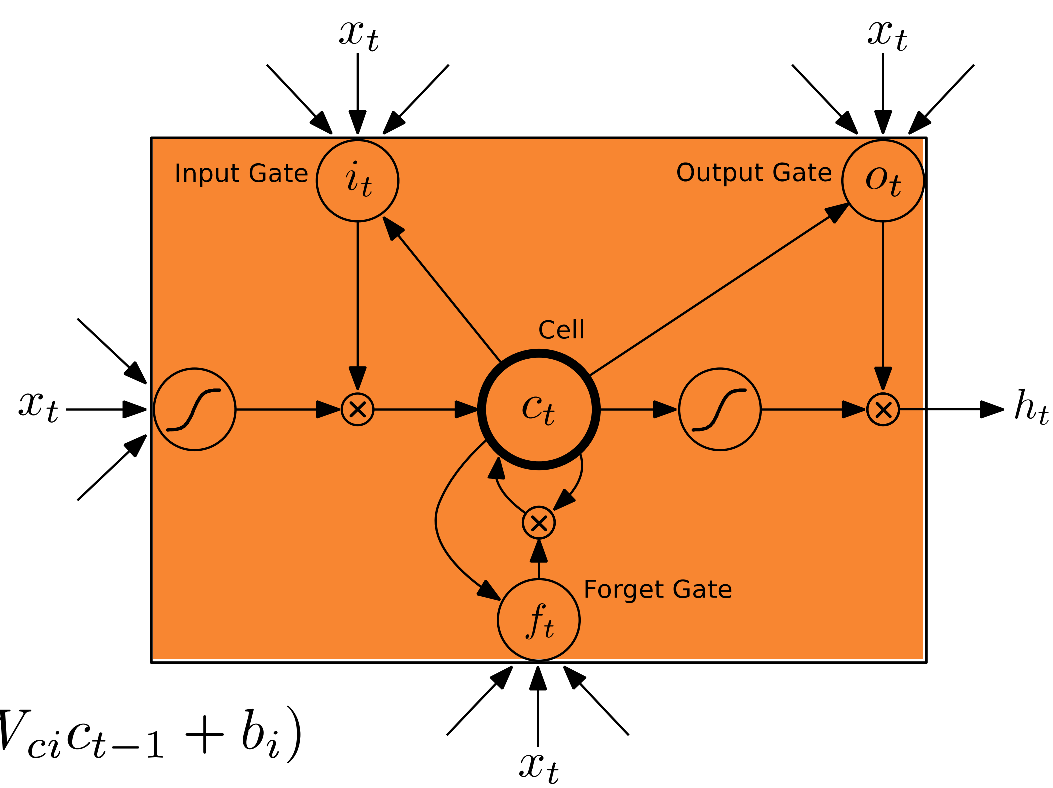


Long Short-Term Memory (LSTM)

- **Input gate:** masks out the standard RNN inputs
- **Forget gate:** masks out the previous cell
- **Cell:** stores the input/forget mixture
- **Output gate:** masks out the values of the next hidden



$$i_t = \sigma\left(W_{xi}x_t + W_{hi}h_{t-1} + W_{ci}c_{t-1} + b_i\right)$$

$$f_t = \sigma\left(W_{xf}x_t + W_{hf}h_{t-1} + W_{cf}c_{t-1} + b_f\right)$$

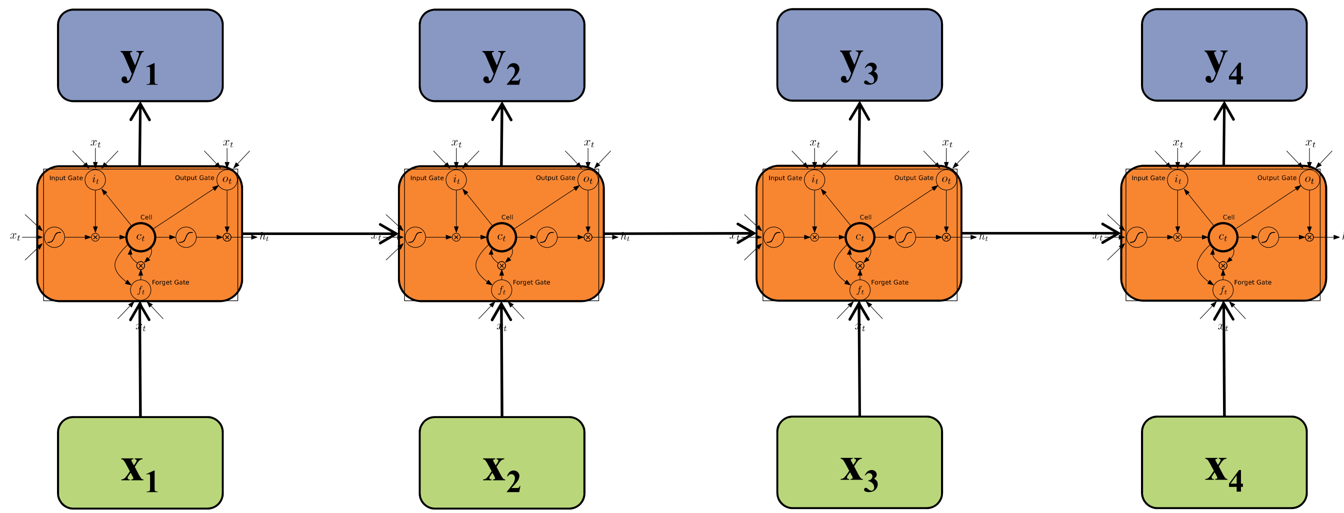
$$c_t = f_t c_{t-1} + i_t \tanh\left(W_{xc}x_t + W_{hc}h_{t-1} + b_c\right)$$

$$o_t = \sigma\left(W_{xo}x_t + W_{ho}h_{t-1} + W_{co}c_t + b_o\right)$$

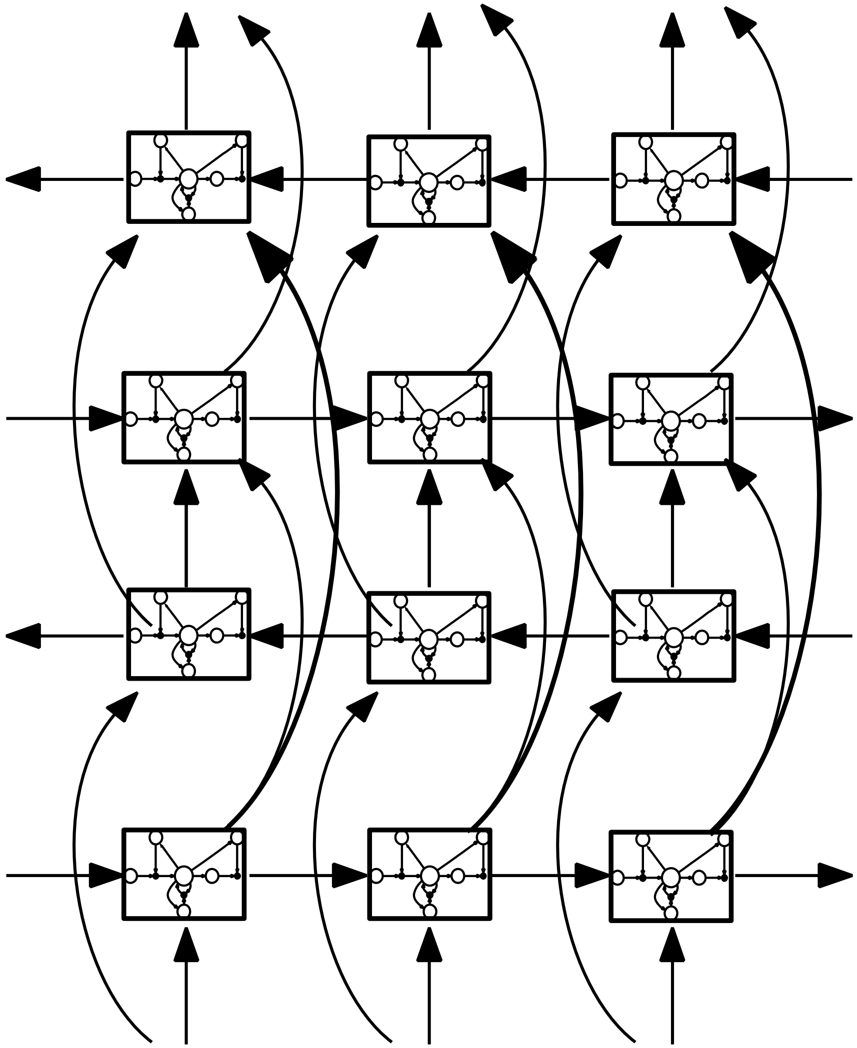
$$h_t = o_t \tanh(c_t)$$

Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)



Deep Bidirectional LSTM (DBLSTM)



- Figure: input/output layers not shown
- **Same general topology** as a Deep Bidirectional RNN, but with **LSTM units** in the hidden layers
- No additional **representational power** over DBRNN, but **easier to learn** in practice

Figure from (Graves et al., 2013)

Deep Bidirectional LSTM (DBLSTM)

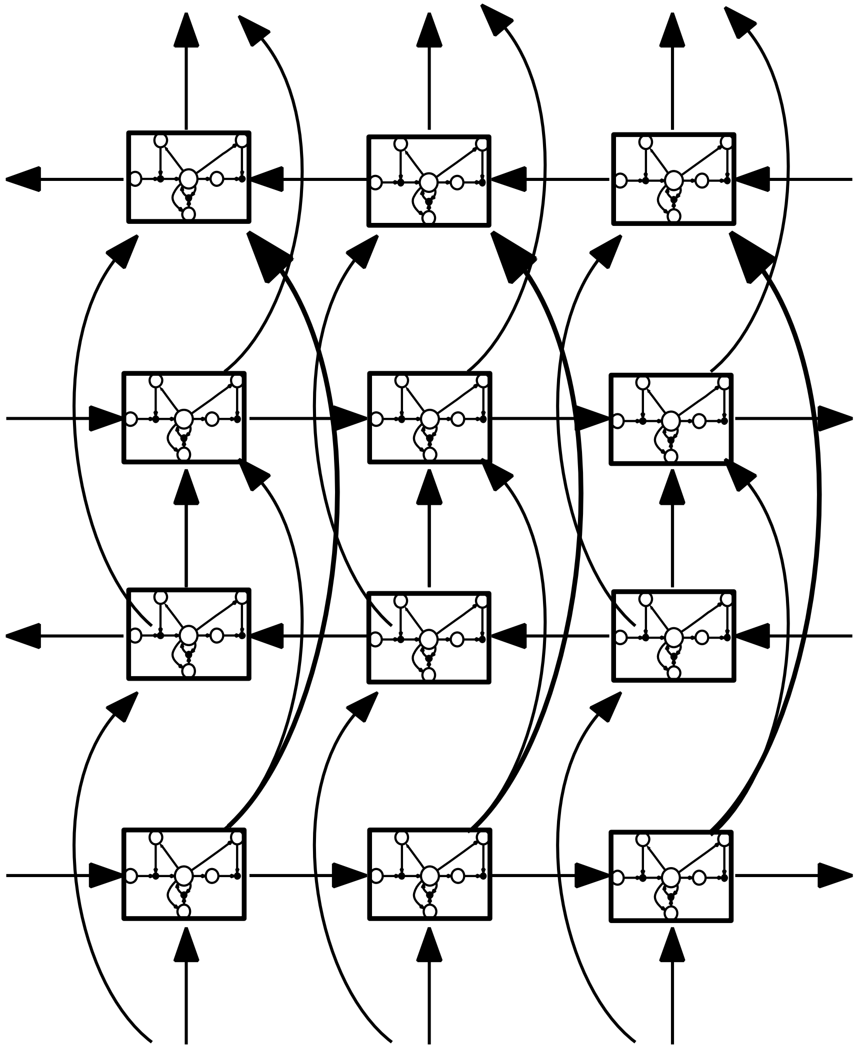


Figure from (Graves et al., 2013)

How important is this particular architecture?

Jozefowicz et al. (2015) **evaluated 10,000 different LSTM-like architectures** and found several variants that worked just as well on several tasks.

RNN Training Tricks

- Deep Learning models tend to consist largely of **matrix multiplications**
- Training tricks:
  - **mini-batching with masking**

	Metric	DyC++	DyPy	Chainer	DyC++ Seq	Theano	TF
RNNLM (MB=1)	words/sec	190	190	114	494	189	298
RNNLM (MB=4)	words/sec	830	825	295	1510	567	473
RNNLM (MB=16)	words/sec	1820	1880	794	2400	1100	606
RNNLM (MB=64)	words/sec	2440	2470	1340	2820	1260	636

  - **sorting into buckets of similar-length sequences,** so that mini-batches have same length sentences
  - **truncated BPTT,** when sequences are too long, divide sequences into chunks and use the final vector of the previous chunk as the initial vector for the next chunk (but don't backprop from next chunk to previous chunk)

Table from Neubig et al. (2017)

RNN Summary

- **RNNs**
  - Applicable to tasks such as **sequence labeling**, speech recognition, machine translation, etc.
  - Able to **learn context features** for time series data
  - Vanishing gradients are still a problem – but **LSTM units** can help
- **Other Resources**
  - Christopher Olah's blog post on LSTMs http://colah.github.io/posts/2015-08-Understanding-LSTMs/