EE 628
Deep Learning
Fall 2019

Lecture 6

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Applied Scientist Sergul Aydore

Amazon Web Services

Overview

- Last lecture we covered
  - Backpropagation
  - Underfitting/Overfitting
- Today, we will cover
  - Optimization Algorithms
  - Convolutional layers

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- Now, it is time to explore common deep learning algorithms in depth
- Almost all problems arising in deep learning are nonconvex
- However, analysis of the algorithms in the context of convex problems can be very instructive.

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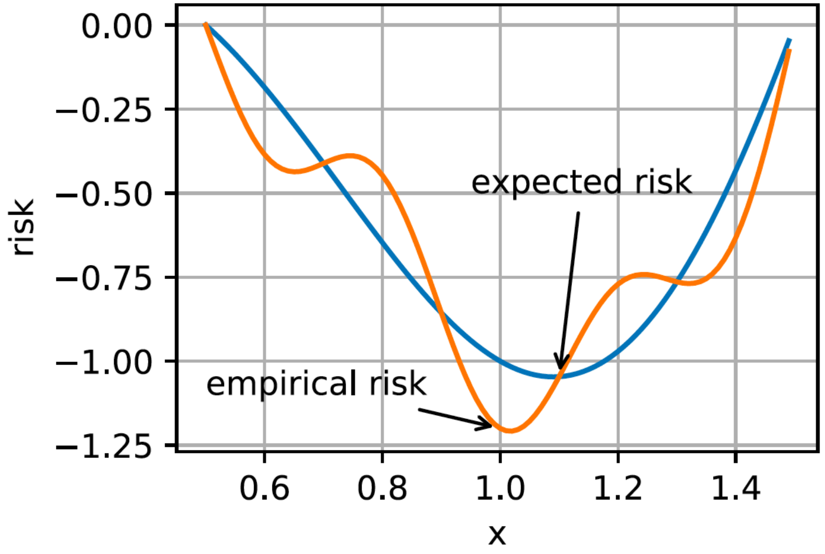

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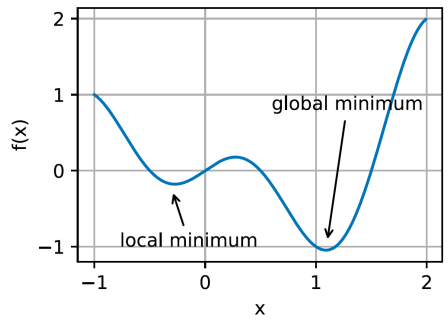

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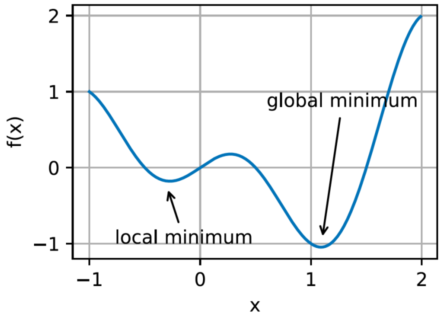

- **Saddle Points:** Any location where all gradients vanish but which is neither a global or a local minimum.
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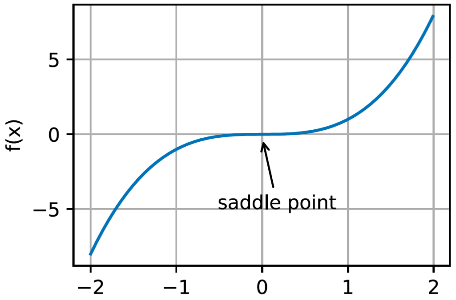

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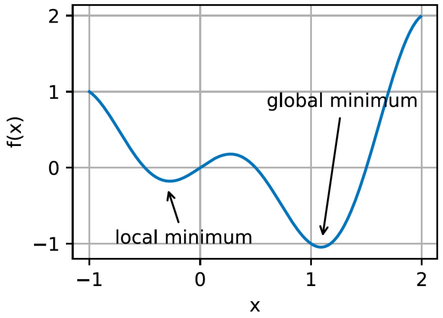

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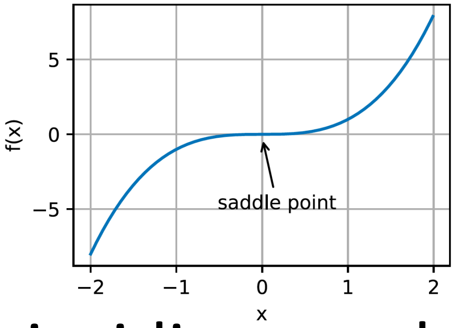

- Vanishing Gradients: Probably, the most insidious problem

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- **Sets**: A set X in a vector space is convex if for any $a, b \in X$ the line segment connecting a and b is also in X. Mathematically, for all $\lambda \in [0, 1]$ we have

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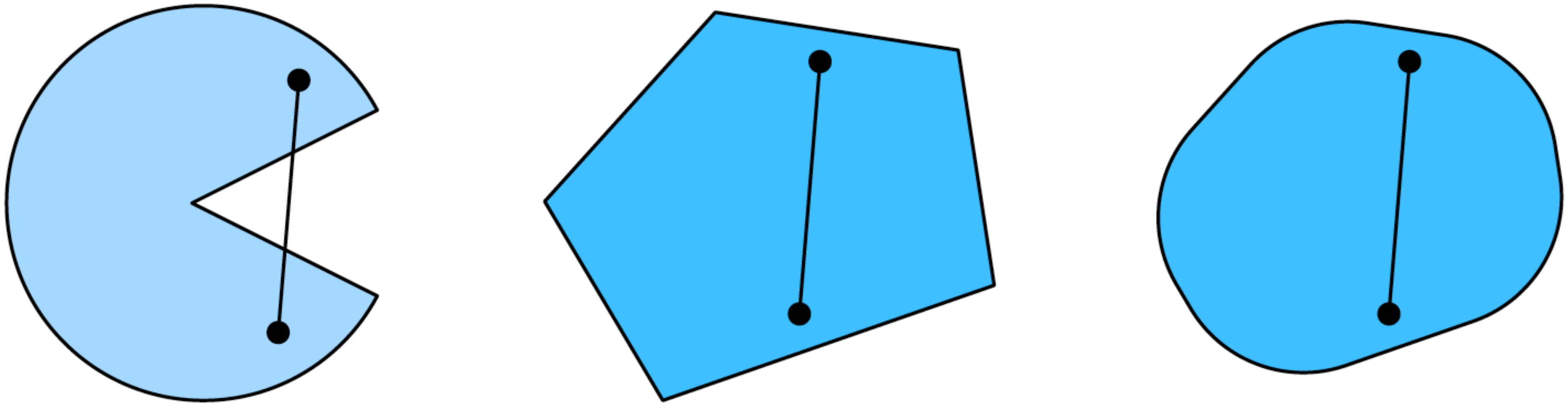

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  - For instance R^d is a convex set
  - In some cases we work with variables of bounded length, such as balls of radius r

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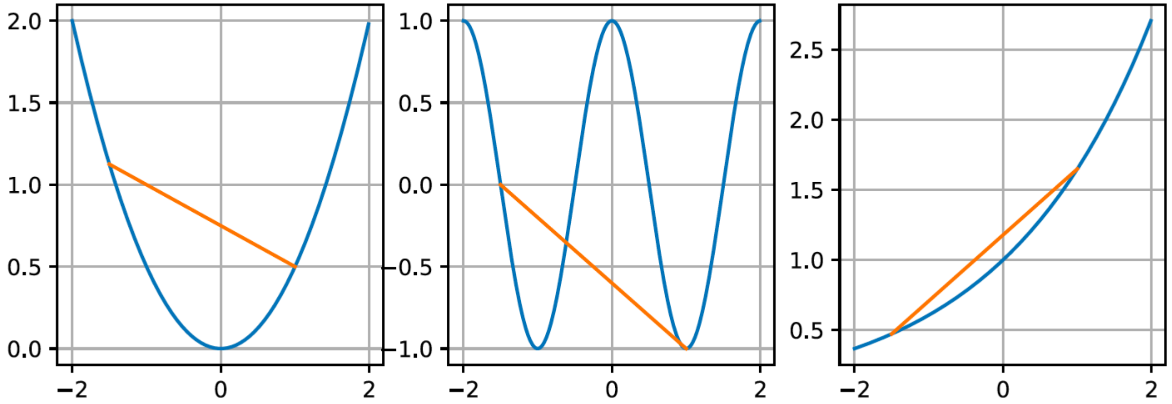
- **Functions**: Given a convex set X, a function defined on it $f: X \to R$ is convex if for all $x, x' \in X$ and for all $\lambda \in [0, 1]$ we have

$$\lambda f(x) + (1 - \lambda) f(x') \geq f(\lambda x + (1 - \lambda) x')$$



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- Jensen's Inequality: It amounts to generalization of the definition of convexity. $\sum_i \alpha_i f(x_i) \geq f\left(\sum_i \alpha_i x_i\right)$ and $\mathrm{E}_x[f(x)] \geq f\left(\mathrm{E}_x[x]\right)$

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- In other words, the expectation of a convex function is larger than the convex function of an expectation.
- Can you prove this?

Gradient Descent

- Let's start with an example in one dimension to explain why the gradient descent algorithm may reduce the value of the objective function.
  - Prove
  - Hint: Use Taylor's series expansion around $x + \epsilon$ and then replace ϵ with $-\eta f'(x)$.

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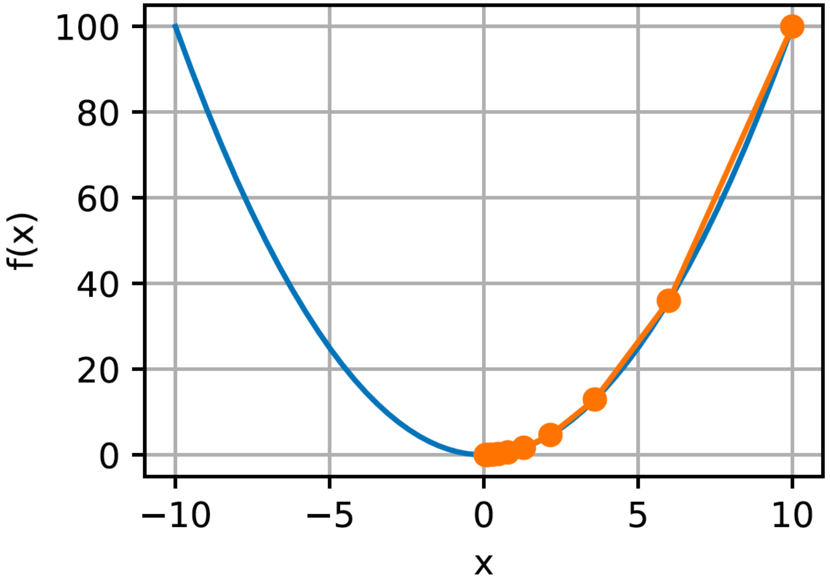
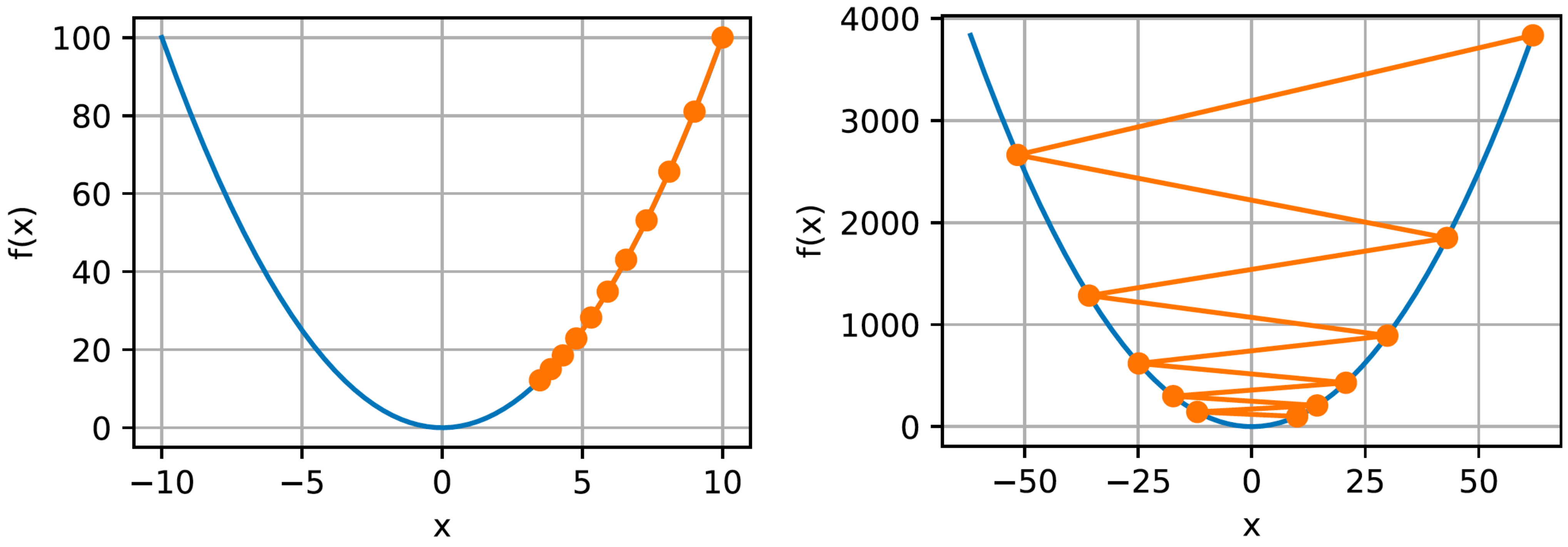


Learning Rate in Gradient Descent

- Which one has large learning rate and which one has small?



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- Choosing a positive learning rate yields the gradient descent algorithm

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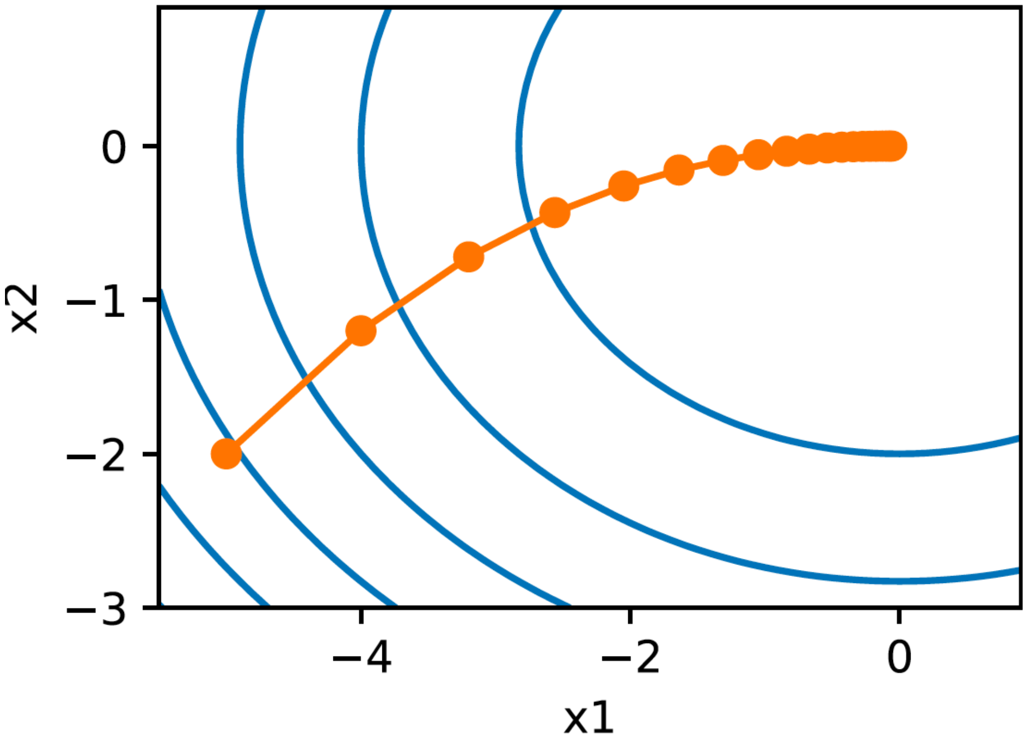

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- What if we determine η automatically?
- Second order methods that also look at the value of *curvature* can help.
- They cannot be applied directly to DL due to computational cost
- But they provide useful intuition into how to design advanced optimization algorithms

Newton’s method

- Reviewing the Taylor expansion of f there is no need to stop after the first term. In fact, we can write it as

$$f(\mathbf{x}+\epsilon) = f(\mathbf{x}) + \epsilon^\top \nabla f(\mathbf{x}) + \frac{1}{2}\epsilon^\top \nabla\nabla^\top f(\mathbf{x})\epsilon + O(\|\epsilon\|^3)$$

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- Consider $f(x) = \frac{1}{2}x^2$, what is the gradient descent rule using Newton’s method?
- Preconditioning: computing the inverse of Hessian is expensive. So only use the diagonal entries of Hessian

Stochastic Gradient Descent (SGD)

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- Computation cost of each update is $\mathcal{O}(n)$
- SGD reduces the computational cost at each iteration
  - At each iteration of SGD, we uniformly sample an index $i \in \{1, \ldots, n\}$ for data instances at random
  - Compute the gradient $\nabla f_i(\mathbf{x})$ to update $\mathbf{x}$

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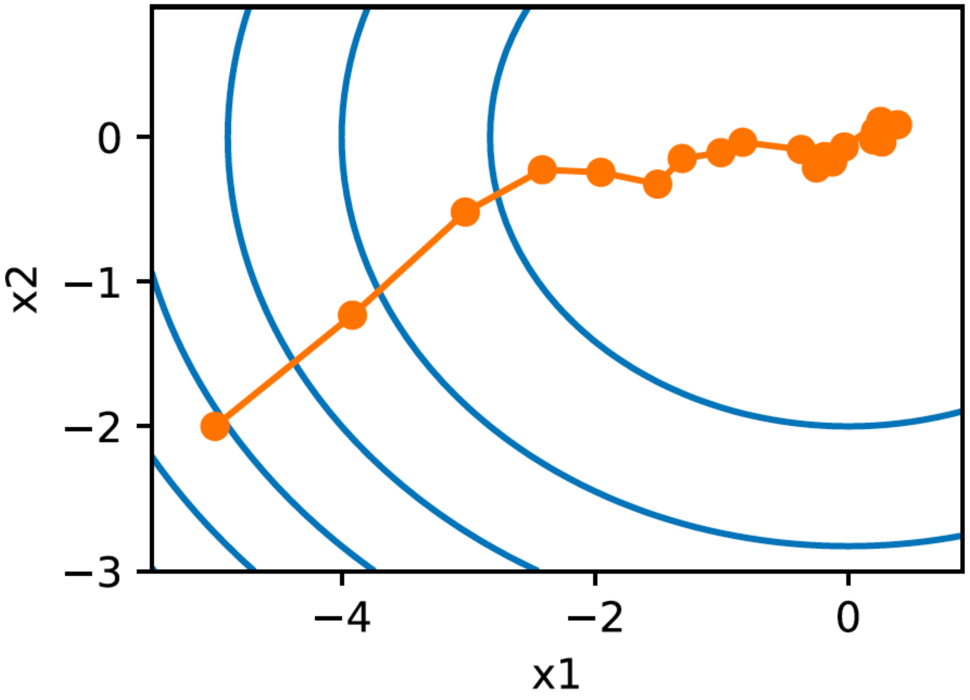
- The trajectory of SGD looks more noisy that GD



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- SGD can self-decay itself by using $\eta_t = \eta t^{\alpha}$ (usually $\alpha = -1$ or $\alpha = -0.5$), $\eta_t = \eta \alpha^t$ (e.g. $\alpha = 0.95$)

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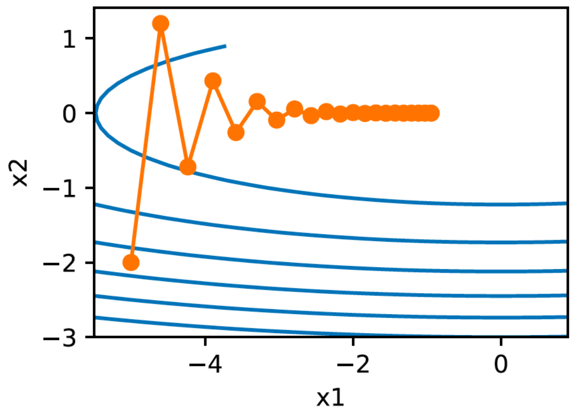
  - Therefore, the variable will move more in Vertical direction



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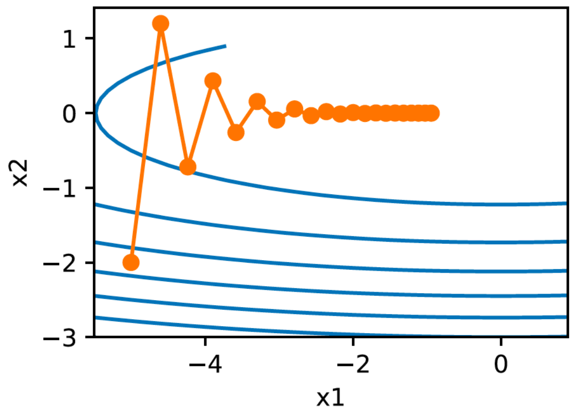

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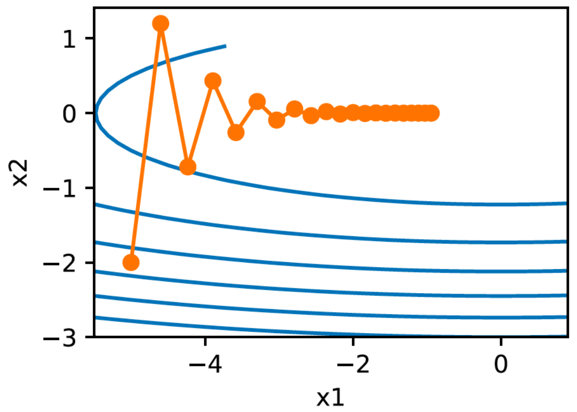

- Small learning rate will cause the variable move slower toward the optimal solution
- Large learning rate will make the variable overshoot in vertical direction

Momentum

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x1

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- At time step $t > 0$, momentum modifies the steps at each iteration as follows

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- When we implement this on the previous example we see that the trajectory is smoother in vertical direction and approaches the optimal solution faster in the horizontal direction.

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- At time step $t > 0$, momentum modifies the steps at each iteration as follows

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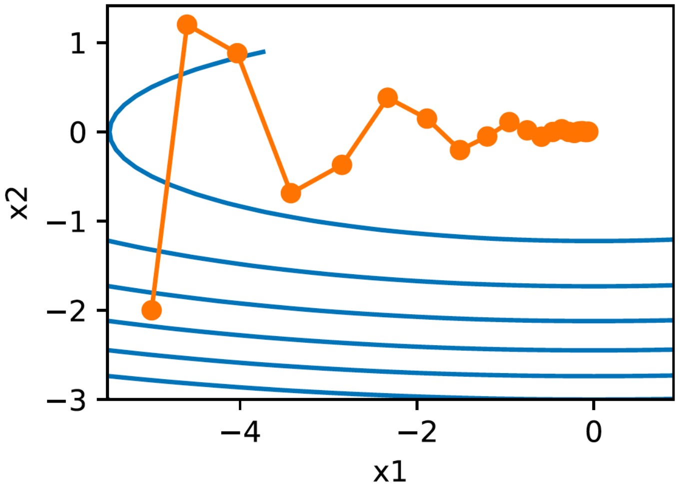
$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \mathbf{v}_t,$$

- When we implement this on the previous example we see that the trajectory is smoother in vertical direction and approaches the optimal solution faster in the horizontal direction.



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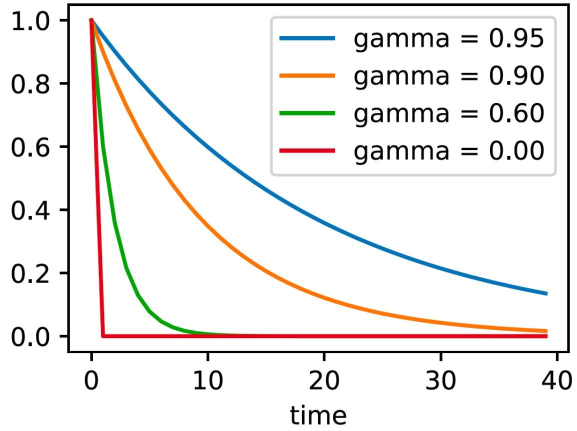

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- The momentum relies on the exponentially weighted moving average to make the direction of the independent variable more consistent
- Now, we introduce Adagrad that adjusts the learning rate according to the gradient value of the independent variable in each direction

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$$\boldsymbol{s}_t \leftarrow \boldsymbol{s}_{t-1} + \boldsymbol{g}_t \odot \boldsymbol{g}_t,$$

- Next, we readjust the learning rate of each element in the independent variable of the objective function using element operations

$$\boldsymbol{x}_t \leftarrow \boldsymbol{x}_{t-1} - \frac{\eta}{\sqrt{\boldsymbol{s}_t + \epsilon}} \odot \boldsymbol{g}_t,$$

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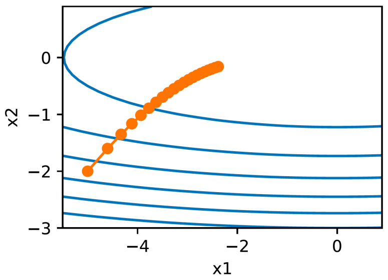
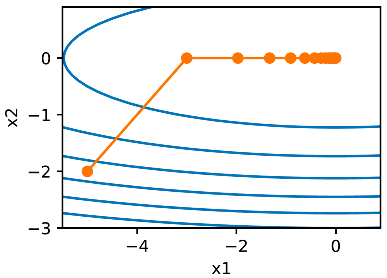
- when the learning rate declines very fast during early iteration, yet the current solution is still not desirable, Adagrad might have difficulty finding a useful solution because the learning rate will be too small at later stages of iteration.
- If we use Adagrad for the example $f(\mathbf{x}) = 0.1\, x_1^2 + 2x_2^2$, we get





Which one uses a larger learning rate?

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- Specifically, given the hyperparameter $0 \leq \gamma < 1$, RMSProp is computed at time step $t > 0$:

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- Like Adagrad, RMSProp readjust the learning rate of each element in the independent variable of the object function as:

$$\mathbf{x}_t \leftarrow \mathbf{x}_{t-1} - \frac{\eta}{\sqrt{\mathbf{s}_t + \epsilon}} \odot \mathbf{g}_t,$$

RMSProp

- If we expand the definition of $\mathbf{s}_t$, we see that:

$$\begin{aligned}
\mathbf{s}_t &= (1-\gamma)\mathbf{g}_t \odot \mathbf{g}_t + \gamma \mathbf{s}_{t-1} \\
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&\cdots \\
&= (1-\gamma)\left(\mathbf{g}_t \odot \mathbf{g}_t + \gamma \mathbf{g}_{t-1} \odot \mathbf{g}_{t-1} + \cdots + \gamma^{t-1} \mathbf{g}_1 \odot \mathbf{g}_1\right).
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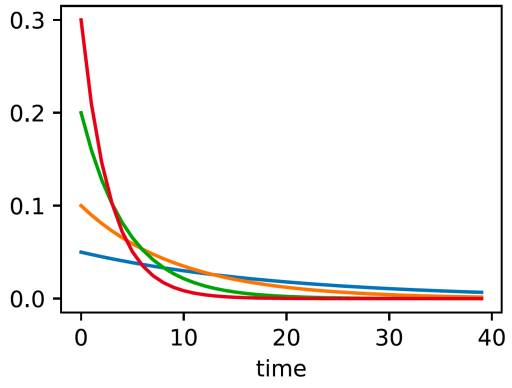
- We visualize these weights in the past 40 time steps for various γ:



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- Next we update the independent variable $\boldsymbol{x}_t \leftarrow \boldsymbol{x}_{t-1} - \boldsymbol{g}'_t.$
- Finally, we use $\Delta\mathbf{x}_t$ to record EWMA on the squares of elements of $\boldsymbol{g}'$

$$\Delta\boldsymbol{x}_t \leftarrow \rho\Delta\boldsymbol{x}_{t-1} + (1-\rho)\boldsymbol{g}'_t \odot \boldsymbol{g}'_t.$$

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- Notice that $\boldsymbol{v}_t = \underbrace{(1-\beta_1)\sum_{i=1}^{t} \beta_1^{t-i}}_{1-\beta_1^t} \boldsymbol{g}_i$ What happens when t is small?
- When t is small, the sum of the mini-batch stochastic gradient weights from each previous time step will be small. To eliminate this effect, we perform bias correction:

$$\hat{\boldsymbol{v}}_t \leftarrow \frac{\boldsymbol{v}_t}{1-\beta_1^t}, \qquad \hat{\boldsymbol{s}}_t \leftarrow \frac{\boldsymbol{s}_t}{1-\beta_2^t}.$$

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- Next, the Adam algorithm will use the bias-corrected variables to re-adjust the learning rate of each element.

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- Ideally, we would find a way to leverage our prior knowledge that nearby pixels are more related to each other.
- Now, we introduce convolutional neural networks (CNNs), a powerful family of neural networks that were designed for precisely this purpose.
- In addition to their strong predictive performance,
  - convolutional neural networks tend to be computationally efficient,
  - both because they tend to require fewer fewer parameters than dense architectures
  - also because convolutions are easy to parallelize across GPU cores

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Constraining the MLP

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- We could formally express this dense layer as follows:

$$h[i,j] = u[i,j] + \sum_{k,l} W[i,j,k,l] \cdot x[k,l] = u[i,j] + \sum_{a,b} V[i,j,a,b] \cdot x[i+a,j+b]$$

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- For any given location (i, j) in the hidden layer $h[i, j]$, we compute its value by summing over pixels in x, centered around (i, j) and weighted by $V[i, j, a, b]$.

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- This is a convolution! We also reduced the number of parameters.

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- This, in a nutshell is the convolutional layer.

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- For two dimensional arrays, we have a corresponding sum with indices (i, j) for f and $(i-a, j-b)$ for g respectively.
- This looks similar to the definition $h[i,j] = u + \sum_{a,b} V[a,b] \cdot x[i+a, j+b]$
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Convolutions

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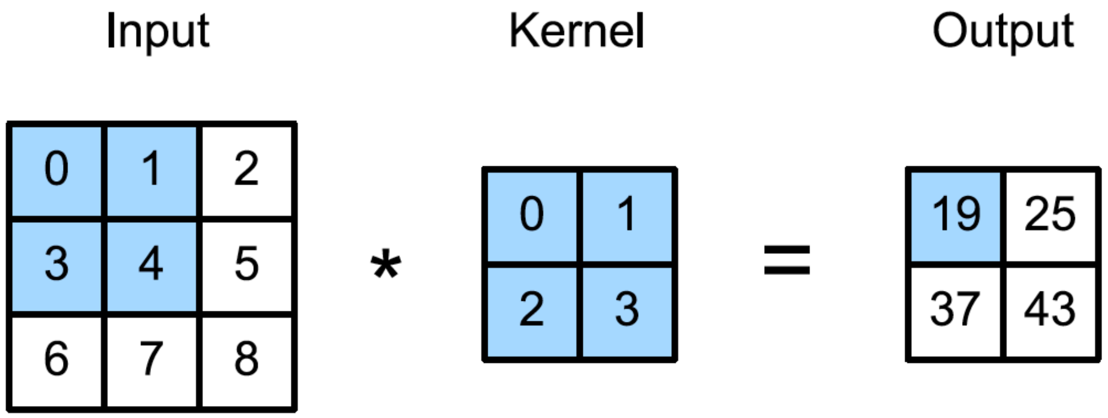
- In order to match the signs, we can use $\tilde{V} = V[-a, -b]$ to obtain $h = x \circledast \tilde{V}$
- Also note that the original definition is actually a *cross-correlation*.

Convolutions for Images

- Let's see how convolutions work in practice.



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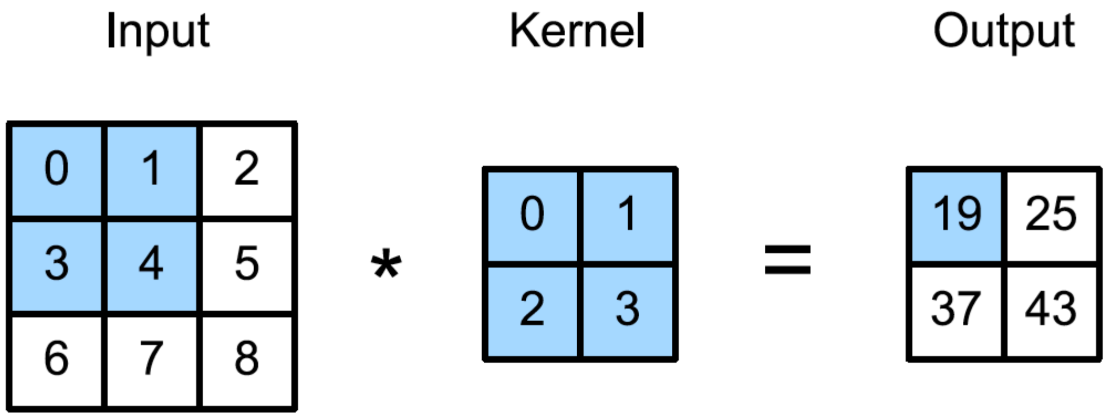

- Start the notebook IN_CLASS_convolutions

Padding and Stride

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  - Solution: **Strides**

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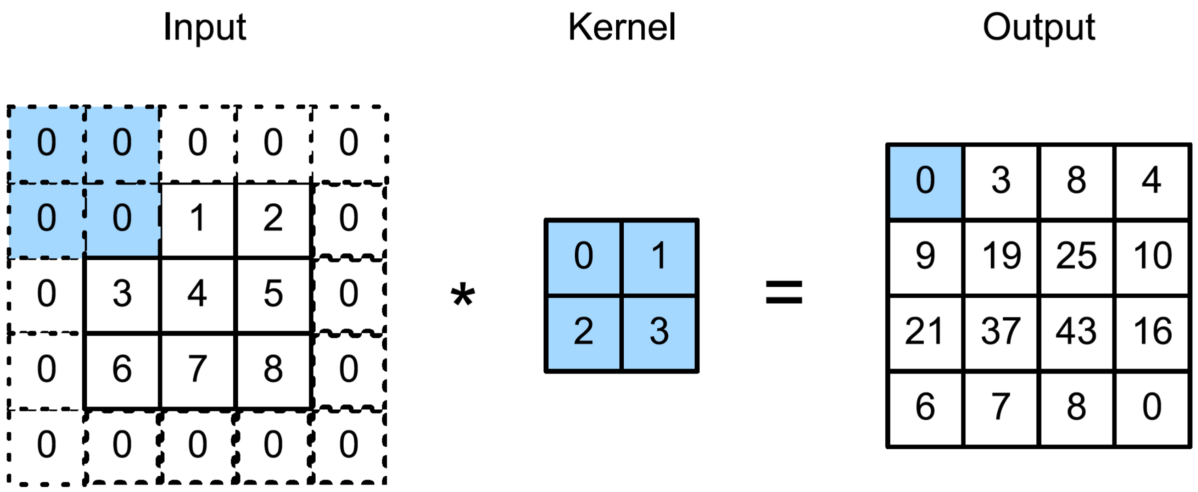

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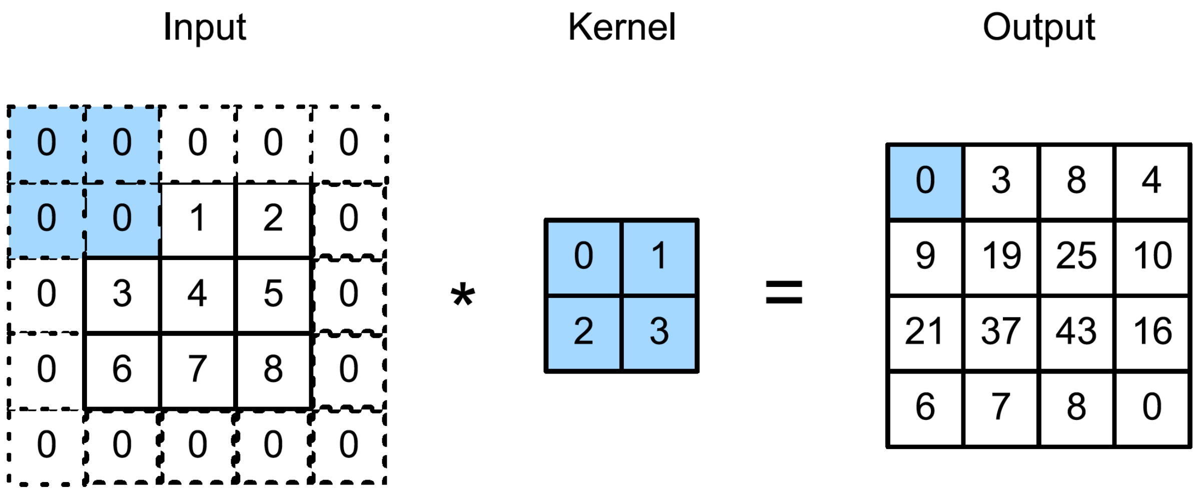

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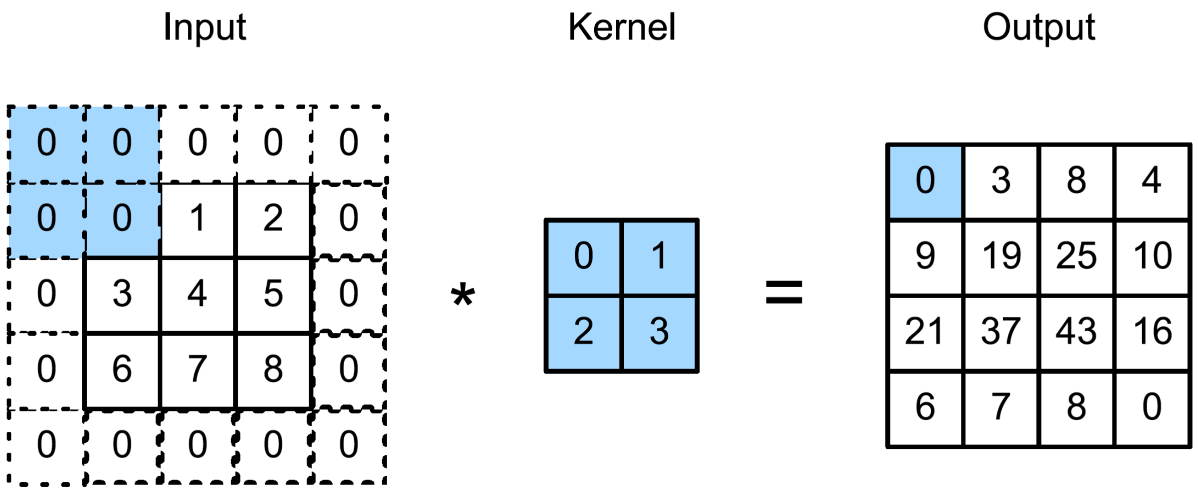

- What is the size of the output after padding?
- What do you think is a good number of padding?

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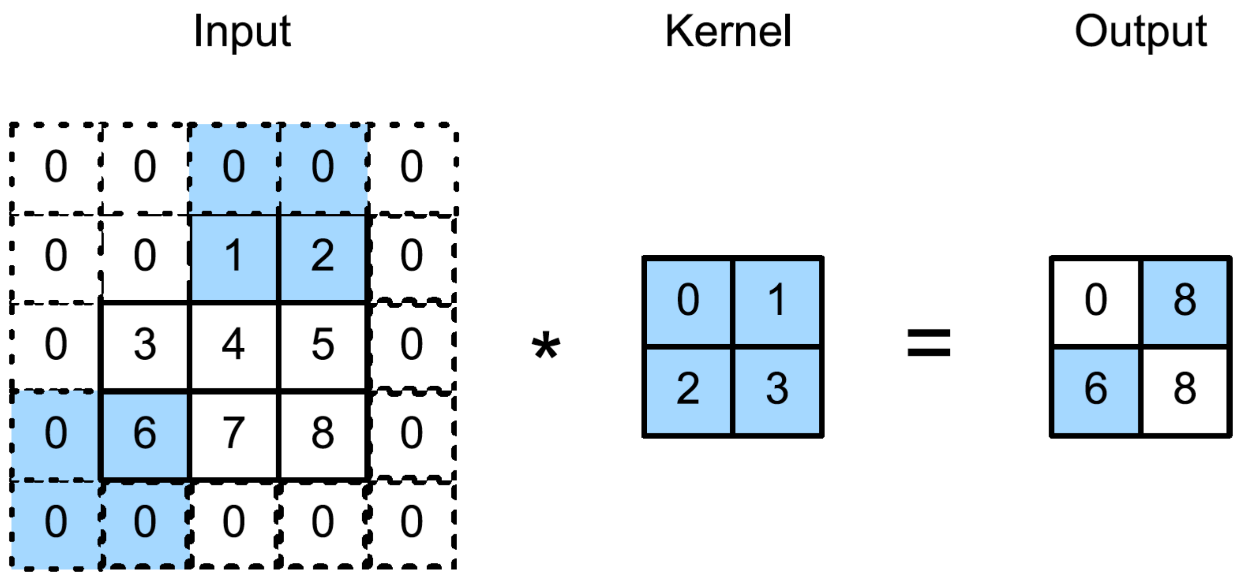
- We refer to the number of rows and columns traversed per slide as the *stride*.



Example for strides with 3 and 2 for height and width, respectively.