COMP 545: Advanced topics in optimization
From simple to complex ML systems

Lecture 4

Overview

- In the last lecture, we:
  - Talked how we can **accelerate** performance in optimization:
    Both in theory (**Newton's method**) and in practice (e.g., **SGD**)
  - Three practical cases: **acceleration, stochasticity, and variance-reduction**
  - Experiments showed advantage of the methods

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    Both in theory (**Newton's method**) and in practice (e.g., **SGD**)
  - Three practical cases: **acceleration, stochasticity, and variance-reduction**
  - Experiments showed advantage of the methods
- Until now, we introduced several hyper-parameters. In this lecture, we will:
  - Discuss what are these **hyper-parameters**
  - Discuss how we can set them correctly or at least heuristically
    in order to **maximize performance**

Gradient descent

- Reminder: how these step size selections are made
- For example, when the objective has **Lipschitz continuous gradients**:

$$f(x_{t+1}) \leq f(x_t) - \eta \left(1 - \frac{\eta L}{2}\right) \cdot \|f(x_t)\|_2^2$$

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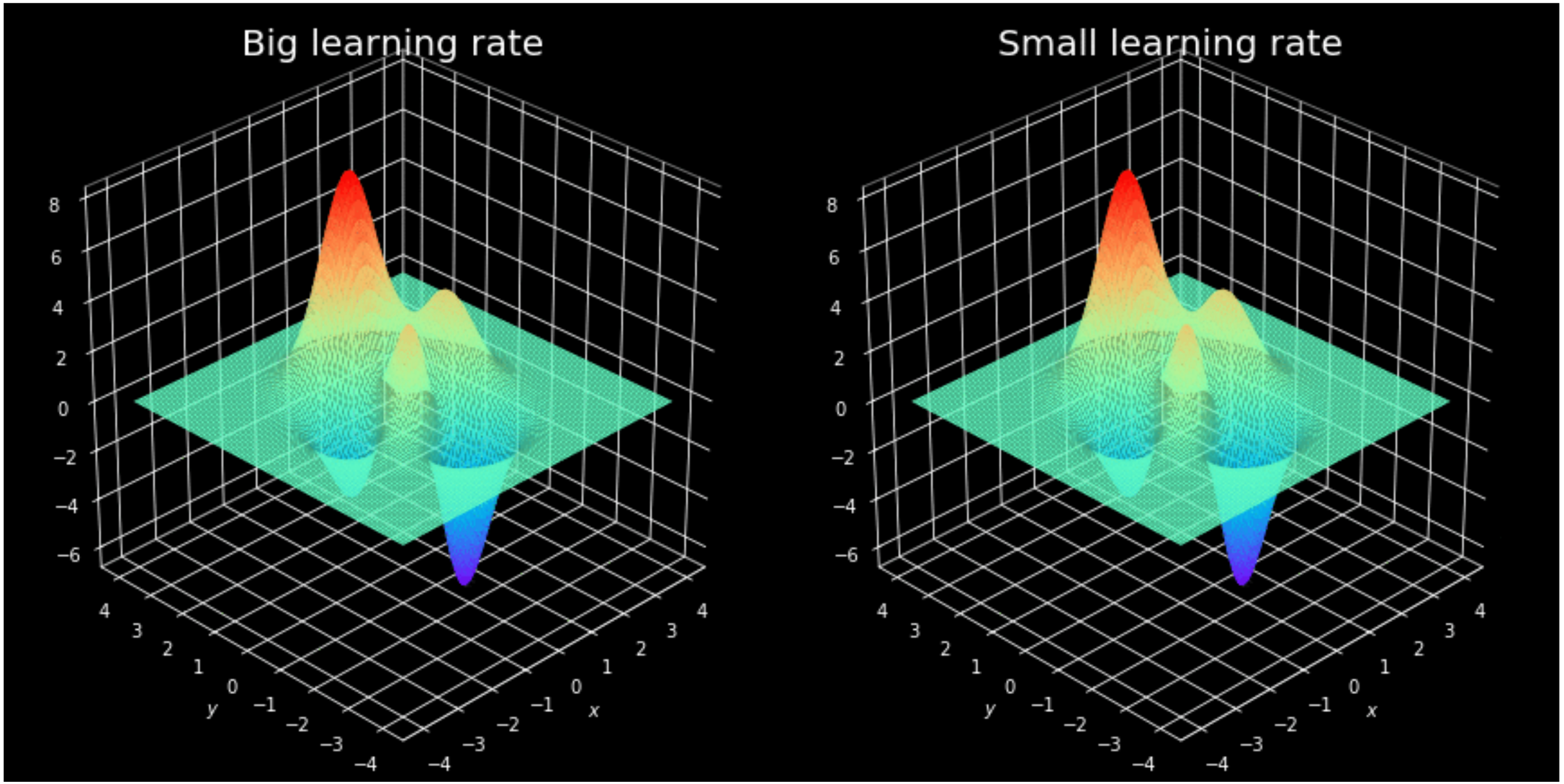
- Using our theory, we obtain:

$$\eta = \frac{1}{L}$$

Gradient descent



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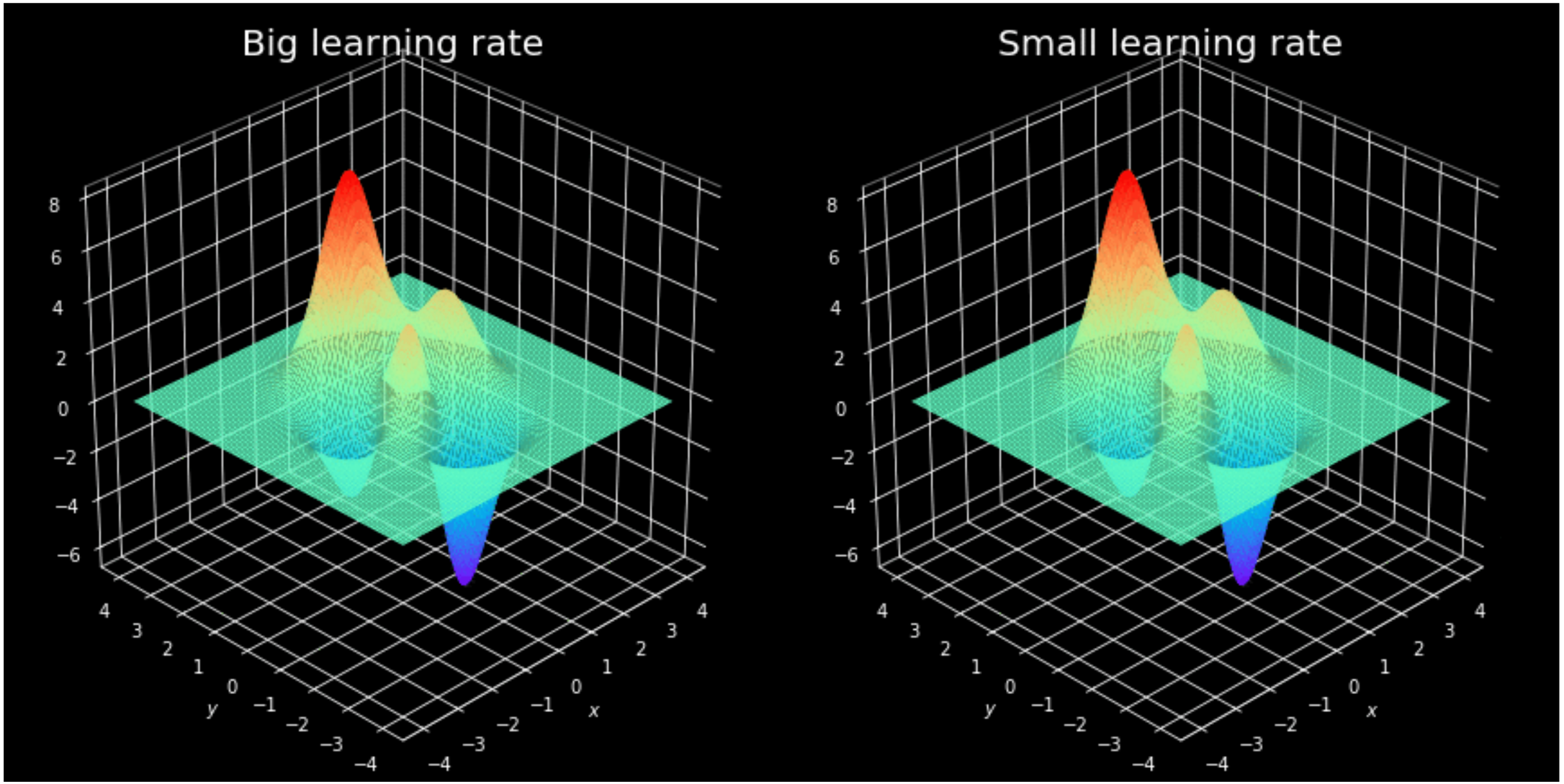

Gradient descent

- How well does $\eta = \frac{1}{L}$ perform?

Demo

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(After all, theory is not that useless..)

Gradient descent

- When the objective has Lipschitz continuous gradients **and** is strongly convex:

$$\|x_{t+1} - x^\star\|_2^2 \leq \left(1 - \frac{2\eta\mu L}{\mu + L}\right) \|x_t - x^\star\|_2^2 + \eta\left(\eta - \frac{2}{\mu + L}\right) \|\nabla f(x_t)\|_2^2$$

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- We then obtain:

$$\eta < \frac{2}{\mu + L}$$

Demo

Projected gradient descent

- We briefly discussed the case of simply-constrained problems
  E.g.,

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & \|x\|_1 \leq \lambda \end{aligned} \qquad \text{or} \qquad \min_x \quad f(x) + \gamma \|x\|_1$$

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- While non-convex objects are harder to optimize, they provide more intuition in tuning: sparsity k or norm-ball radius λ?

There is statistical theory for this selection

Initialization in gradient descent

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- We will see later in the course that initialization plays a key role in more involved scenaria

Newton's method

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(Similar strategies for L-BFGS)

(Disclaimer: this is a very rough description. There are many rules that one can use to determine whether to increase/decrease the step size (backtracking line search, Armijo rule, using Newton's decrement, etc). There is also theory that characterizes when we leave the linear rate and we enter the quadratic convergence rate)

Stochastic gradient descent

- So far, the stochastic method we discussed is SGD (More to come!)

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- For **step size**, there are various schedules:

(More often than not, step size is called "learning rate")

1. Constant step size

$$\eta_t \equiv \eta = c \quad (\text{usually } c = 0.1)$$

Demo

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2. Inverse time decay

$$\eta_t = \frac{\eta}{1 + ct}$$

Step size (as if it was constant step size)

Constant c

Demo

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3. Step decay

$$\eta_t = \eta \cdot q^{(1+e)/k}$$

Step size (as if it was constant step size)

E.g., q = 0.5, e is the epoch number, k = 10

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    (We want to explore better around that area)

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- Theoretically (convex), **mini-batch SGD decreases error** by a factor $|\mathcal{I}_t|$ compared to standard SGD
- For larger batch sizes, **mini-batch SGD allows more parallelism**

(To be discussed in future lectures)

Large-batch training

(On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima - Extra slides)

- Main drawback of SGD: sequential

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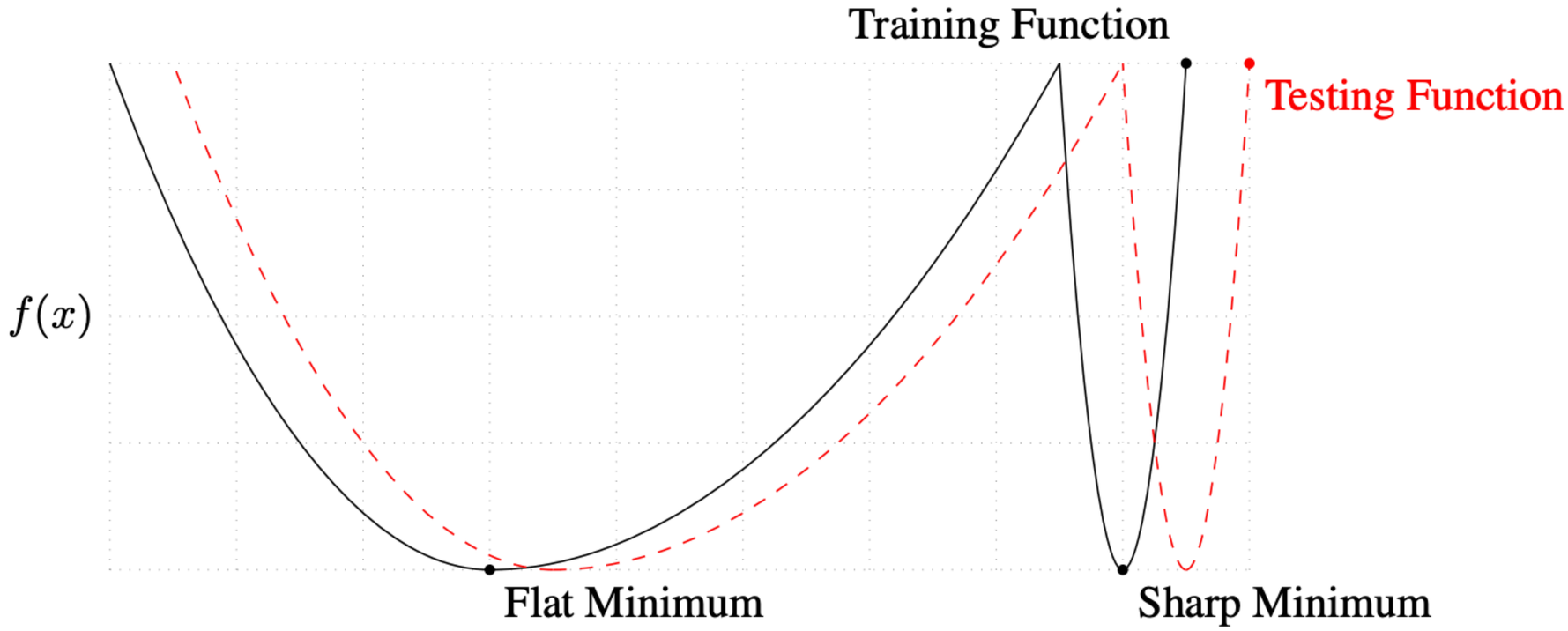

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Name	Network Type	Architecture	Data set
F_1	Fully Connected	Section B.1	MNIST (LeCun et al., 1998a)
F_2	Fully Connected	Section B.2	TIMIT (Garofolo et al., 1993)
C_1	(Shallow) Convolutional	Section B.3	CIFAR-10 (Krizhevsky & Hinton, 2009)
C_2	(Deep) Convolutional	Section B.4	CIFAR-10
C_3	(Shallow) Convolutional	Section B.3	CIFAR-100 (Krizhevsky & Hinton, 2009)
C_4	(Deep) Convolutional	Section B.4	CIFAR-100

Table 2: Performance of small-batch (SB) and large-batch (LB) variants of ADAM on the 6 networks listed in Table 1

	Training Accuracy		Testing Accuracy	
Name	SB	LB	SB	LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
C_2	$99.99\% \pm 0.04\%$	$99.99\% \pm 0.01\%$	$89.24\% \pm 0.12\%$	$87.26\% \pm 0.07\%$
C_3	$99.56\% \pm 0.44\%$	$99.88\% \pm 0.30\%$	$49.58\% \pm 0.39\%$	$46.45\% \pm 0.43\%$
C_4	$99.10\% \pm 1.23\%$	$99.57\% \pm 1.84\%$	$63.08\% \pm 0.5\%$	$57.81\% \pm 0.17\%$

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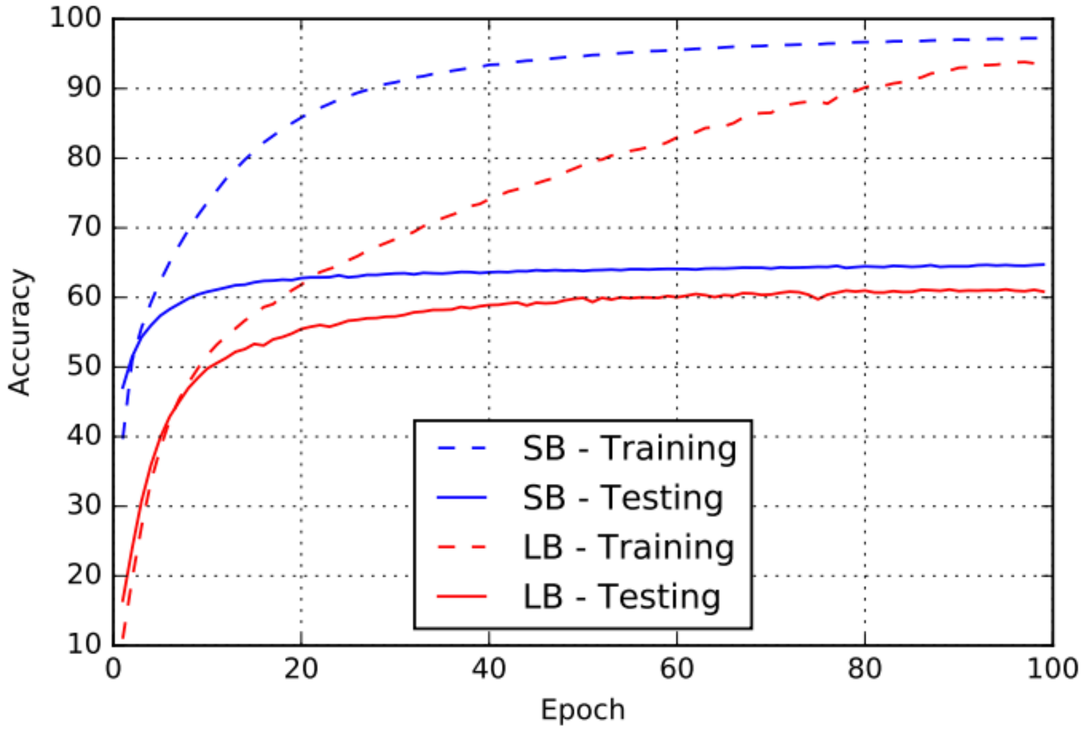
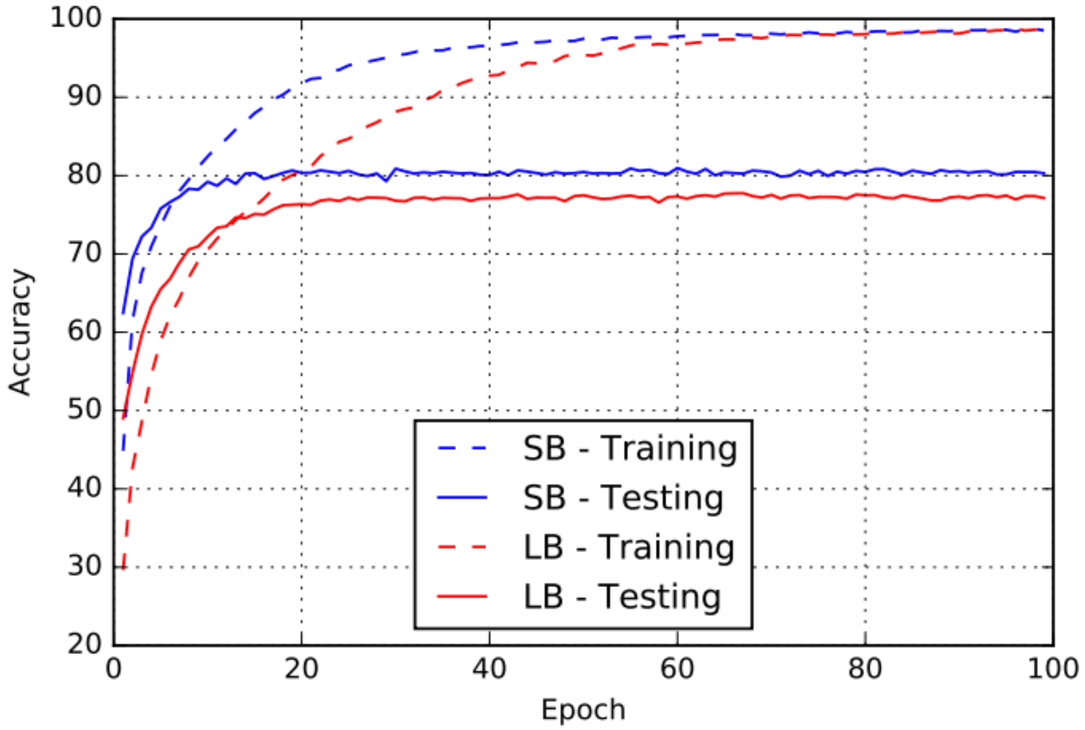


(a) Network F_2



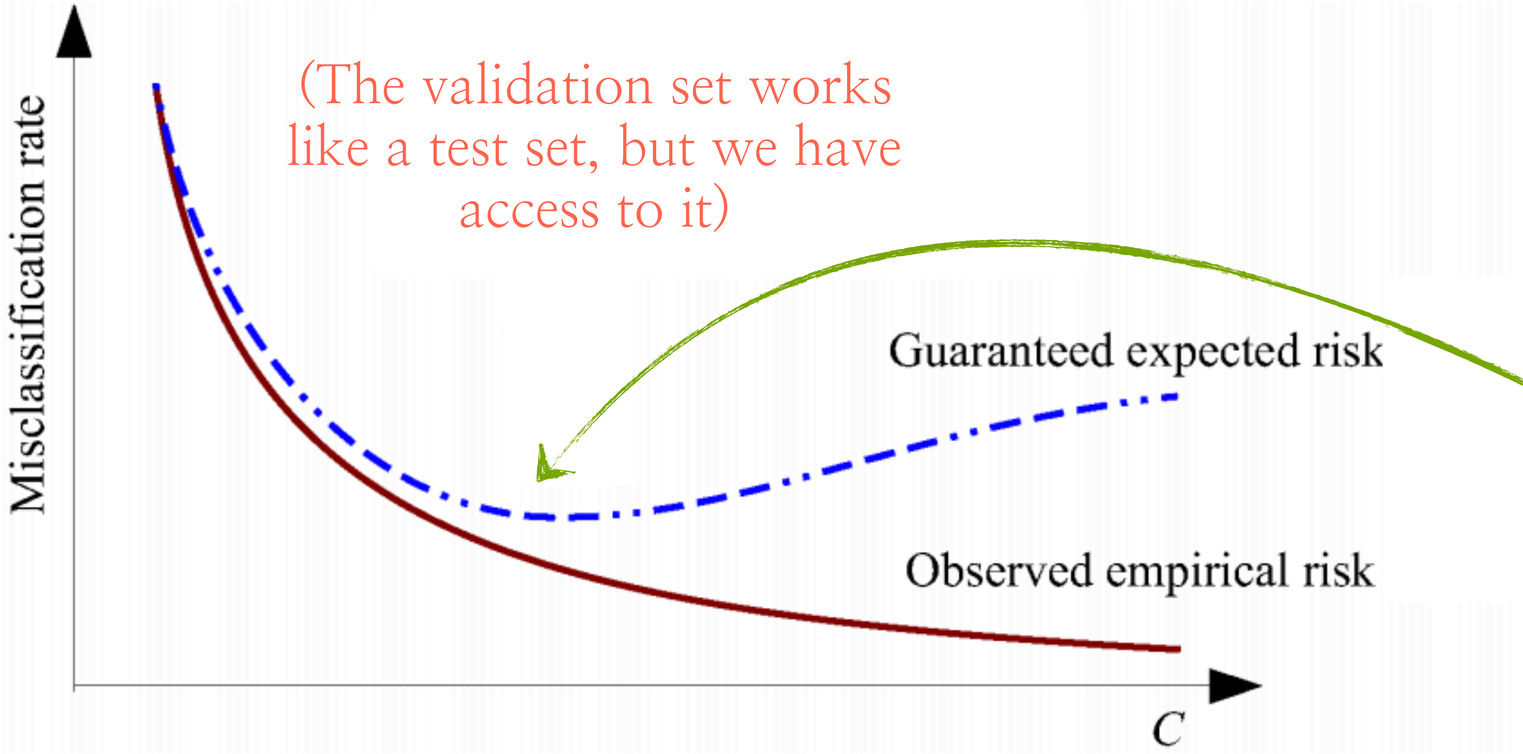
(b) Network C_1

Early stopping

(Requires a bit of detour)

- In machine learning, our aim is to make an algorithm perform well on training data (we study this already), but **also on unseen input.**

(This is the distinction between training error and test error)



- While training error keeps decreasing, our performance on unseen data deteriorates

- This motivates the use of a validation set

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- Early stopping does not damage or alter the learning dynamics (compare with explicit regularization techniques that change the objective)

- There is a connection of early stopping with that of ℓ_2-norm reg.

- However, it does not need hyper-parameter tuning

Early stopping

- Since early stopping requires part of the training data, we can use the following meta-algorithm:

Algorithm A meta-algorithm for using early stopping to determine how long to train, then retraining on all the data.

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Set $\boldsymbol{\theta}$ to random values again.
Train on $\boldsymbol{X}^{(\text{train})}$ and $\boldsymbol{y}^{(\text{train})}$ for i^* steps.

Conclusion

- This short lecture was about **hyper-parameter tuning**
- However, we only scratched the surface of hyper-parameter tuning; more to come in future lectures
- Key observation (even in these simplified scenaria) is that tuning can be even more important than which algorithm to use

Next lecture

- Sparse model selections and non-convex hard thresholding