Lecture 1: Regression

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Open in Colab

Prince (2023, chaps. 2, 6, 8).[1]

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Linear Regression

Prince (2023, chap. 2)

Linear Model

$$\mathbf{y} = \mathbf{X}\beta + \varepsilon$$

Minimizing the mean-squared error (MSE)

$$\min_{\beta} \frac{1}{n}(y - X\beta)^T(y - X\beta)$$

Minimizing MSE Loss (2.1-2.3)

Analytical Solution

$$\min_{\beta} \frac{1}{n}(y - X\beta)^T(y - X\beta)$$

Setting the gradient with respect to β to zero

$$0 = \nabla_{\beta}[y^T y - 2\beta^T X^T y + \beta^T X^T X\beta] = -2X^T y + 2X$$

yields the BLUE estimator (Gauss-Markov)

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

scikit-learn

scikit-learn

```
1 from sklearn.linear_model import LinearRegression
2 model = LinearRegression()
3 model.fit(X_train, y_train)
4 print(model.coef_[2], model.intercept_)
```

```
546.1898661888232 152.05949984245817
```

```
Text(0, 0.5, 'Diabetes Risk')
```

Model Fitting & Optimization

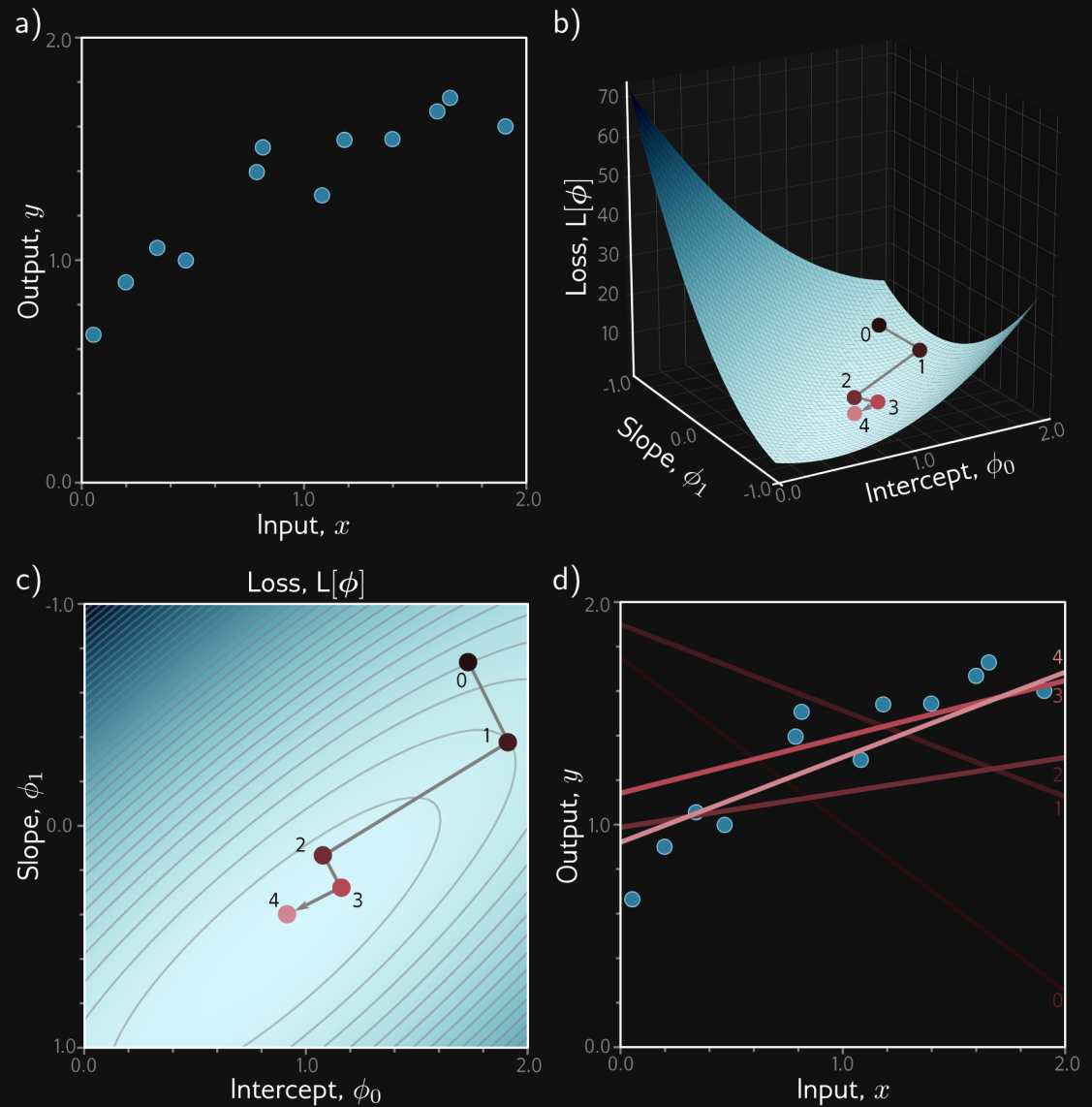
$$\hat{\phi} = \arg\min_{\phi} L(\phi)$$

Prince (2023, chap. 6)

Gradient Descent[1]

$$\phi \leftarrow \phi - \alpha \nabla_{\phi} L(\phi)$$

where α fixed learning rate or line search.



1. Cauchy (1847)

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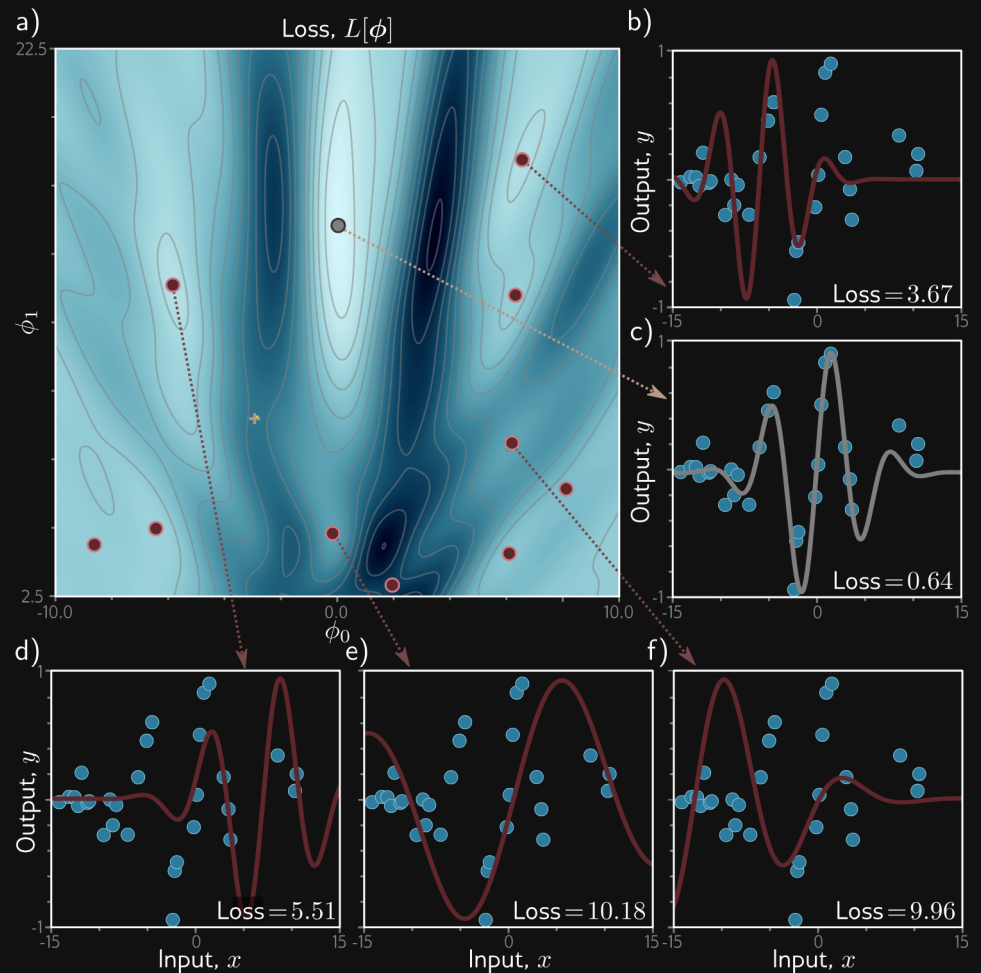
Nonlinear Model

Loss functions generally non-convex, possibly multiple local minima.



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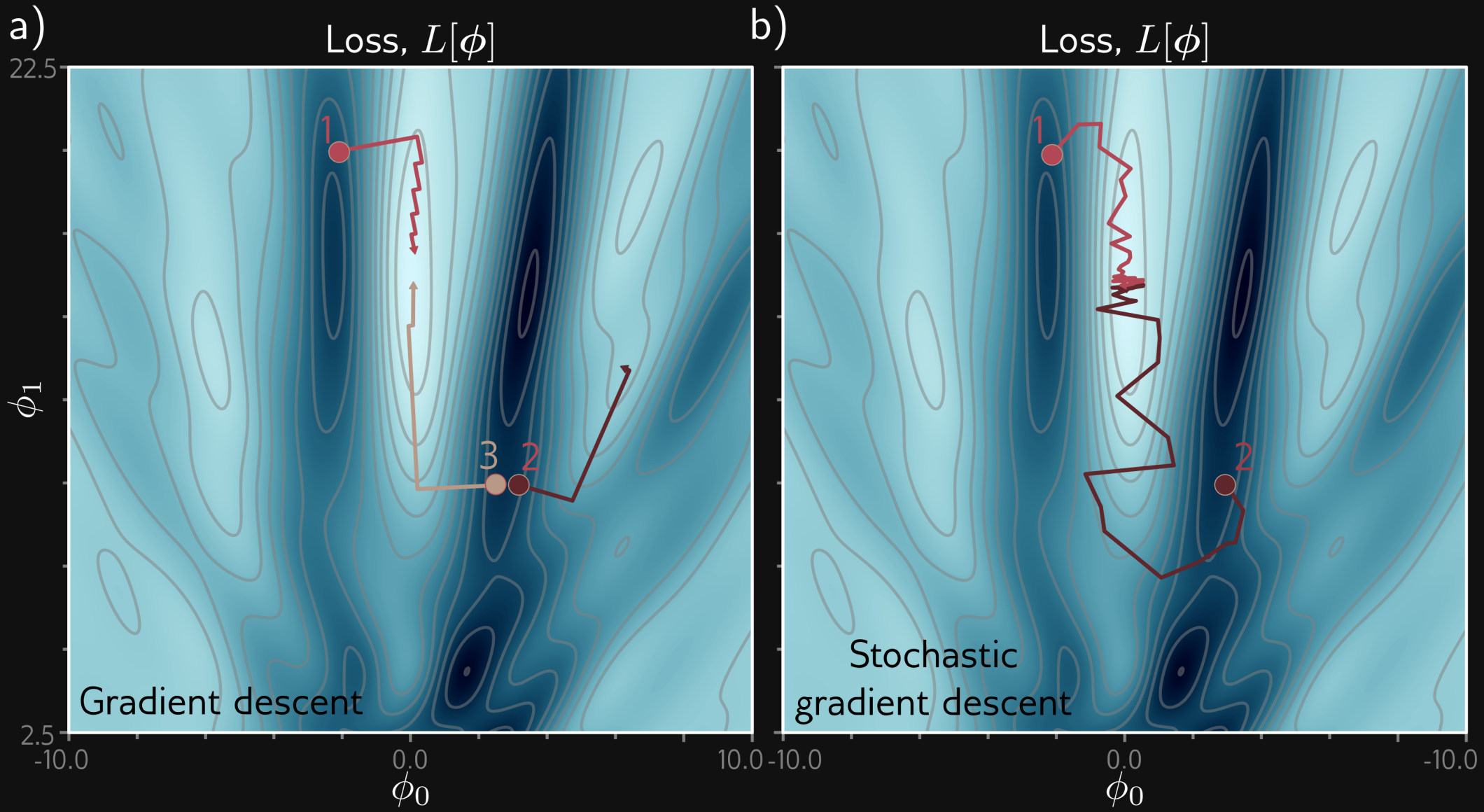
Stochastic Gradient Descent

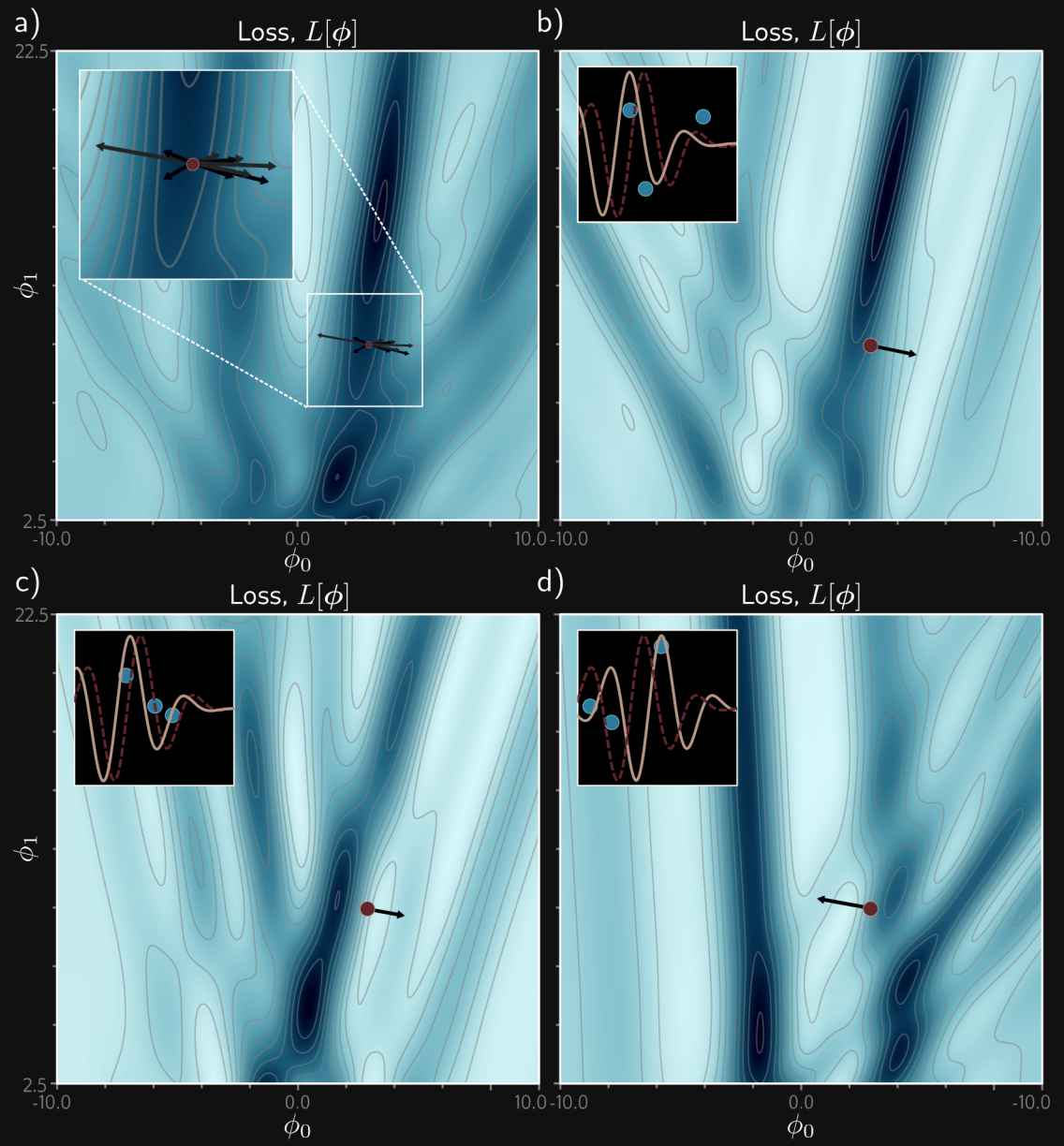


Stochastic Gradient Descent [1]

Compute gradient on a mini-batch B_t of data points

$$\phi_{t+1} \leftarrow \phi_t - \alpha \sum_{i \in B_t} \nabla_\phi l_i(\phi_t; x_i, y_i)$$

- Sampled without replacement within each epoch (sweep of training data).
- Learning rate often decreasing over time.



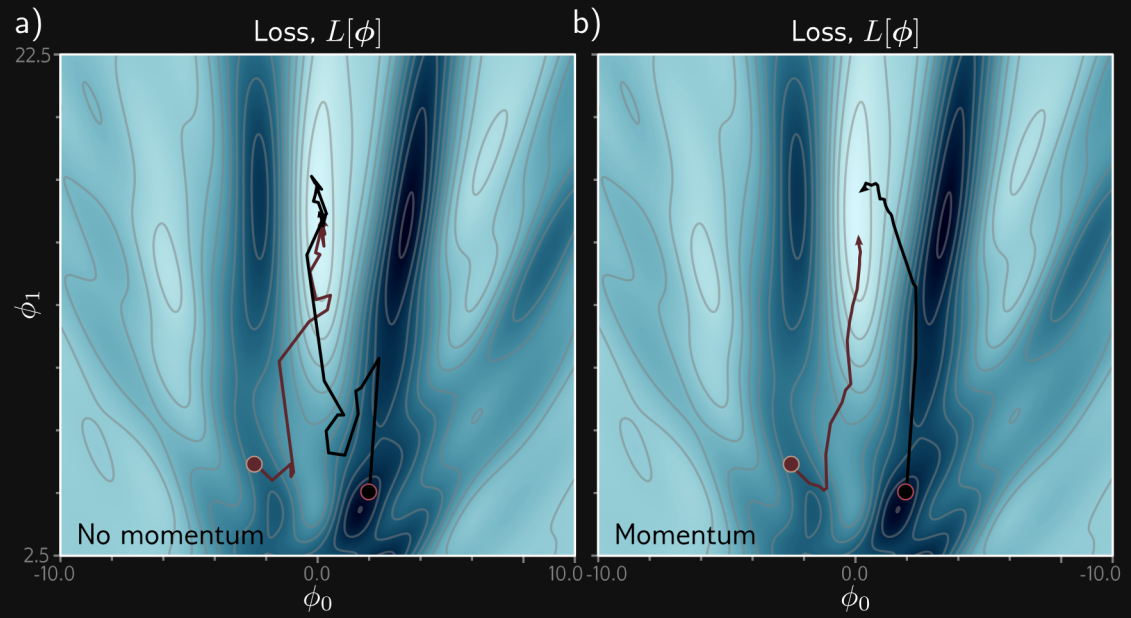
1. Robbins & Monro (1951)

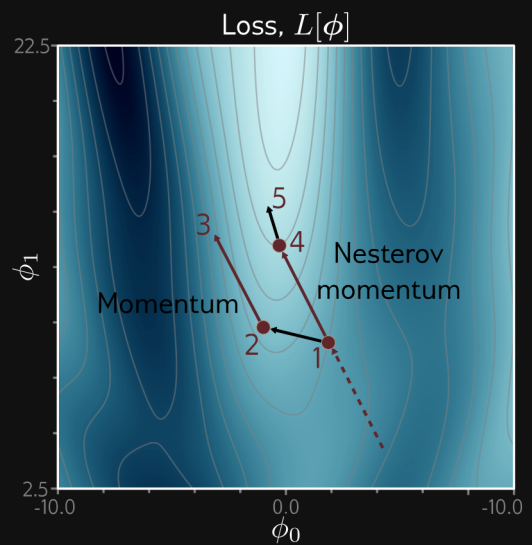
Nesterov Accelerated Momentum [1]

$$m_{t+1} \leftarrow \beta m_t + (1-\beta) \sum_{i \in B_t} \nabla_\phi l_i(\phi_t - \alpha\beta m_t; x_i, y_i)$$

$$\phi_{t+1} \leftarrow \phi_t - \alpha m_{t+1}$$

adds momentum (m_t) *before* evaluating gradient.





1. Nesterov (1983)

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Adaptive Moment Estimation (Adam) [1]

Normalizes the gradient while relying on momentum to avoid convergence issues.

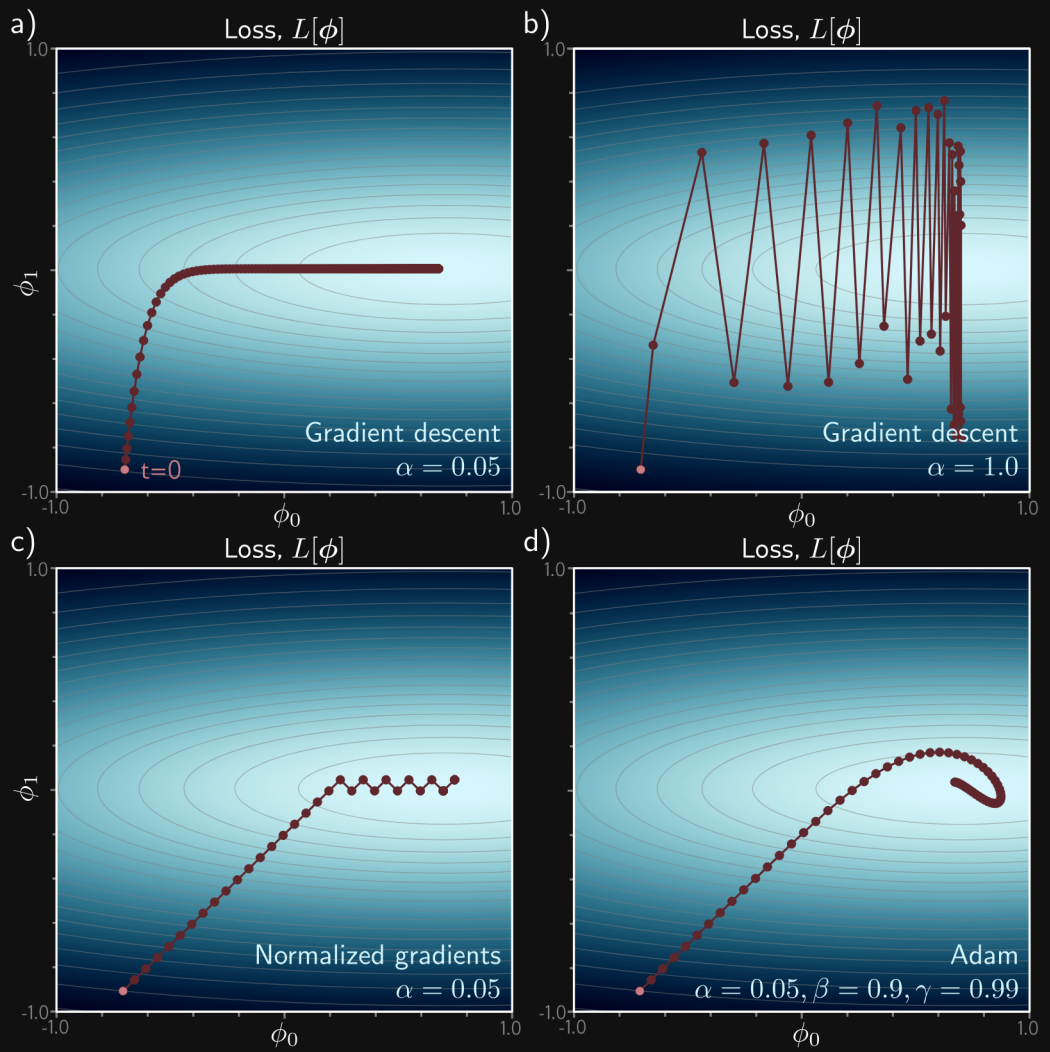
$$m_{t+1} \leftarrow \beta m_t + (1-\beta) \sum_{i \in B_t} \nabla_\phi l_i(\phi_t; x_i, y_i)$$

$$v_{t+1} \leftarrow \gamma v_t + (1-\gamma) \left(\sum_{i \in B_t} \nabla_\phi l_i(\phi_t; x_i, y_i) \right)^2$$

$$\phi_{t+1} \leftarrow \phi_t - \alpha \frac{\frac{m_{t+1}}{1-\beta^{t+1}}}{\sqrt{\frac{v_{t+1}}{1-\gamma^{t+1}}} + \epsilon}$$

1. Kingma & Ba (2015)

Adaptive Moment Estimation (Adam)



PyTorch

PyTorch

Setup

```
 1 import torch
 2 from torch import nn
 3 import torch.optim as optim
 4 from torchvision import datasets
 5 from torch.utils.data import DataLoader
 6 from torchvision.transforms import ToTensor, Compose, Grayscale
 7 import random
 8
 9 if torch.backends.mps.is_available():
10   DEVICE = torch.device("mps") # Apple Silicon Metal Performance Shaders
11 elif torch.cuda.is_available():
12   DEVICE = torch.device("cuda") # GPU
13 else:
14   DEVICE = torch.device("cpu") # CPU
```

Key components:

Tensors

Tensors “live” on a device

```
1 X_train = torch.tensor(X.values, dtype=torch.float32).to(DEVICE)
2 y_train = torch.tensor(y.values, dtype=torch.float32).to("cpu")
3 print(X_train.device)
4 X_train =X_train.to("cpu")
5 print(X_train.device)
```

```
mps:0
cpu
```

The Previous Regression

```
1 solution = torch.linalg.lstsq(X_train, y_train)
2 coefficients = solution.solution[:-1].flatten()  # All coefficients except
3 intercept = solution.solution[-1].item()  # Intercept
4 print(coefficients[2], intercept)
```

```
tensor(519.8459) 152.13348388671875
```

The Previous Regression

```python
class LinearRegressionModel(nn.Module):
    def __init__(self, input_dim):
        super(LinearRegressionModel, self).__init__()
        self.linear = nn.Linear(input_dim, 1)

    def forward(self, x):
        return self.linear(x)

model = LinearRegressionModel(input_dim=X_train.shape[1])
criterion = nn.MSELoss()
# optimizer = optim.SGD(model.parameters(), lr=0.01)
optimizer = optim.Adam(model.parameters(), lr=0.01)

# Training loop
epochs = 15000
for epoch in range(epochs):
    # Forward pass
    outputs = model(X_train)
```

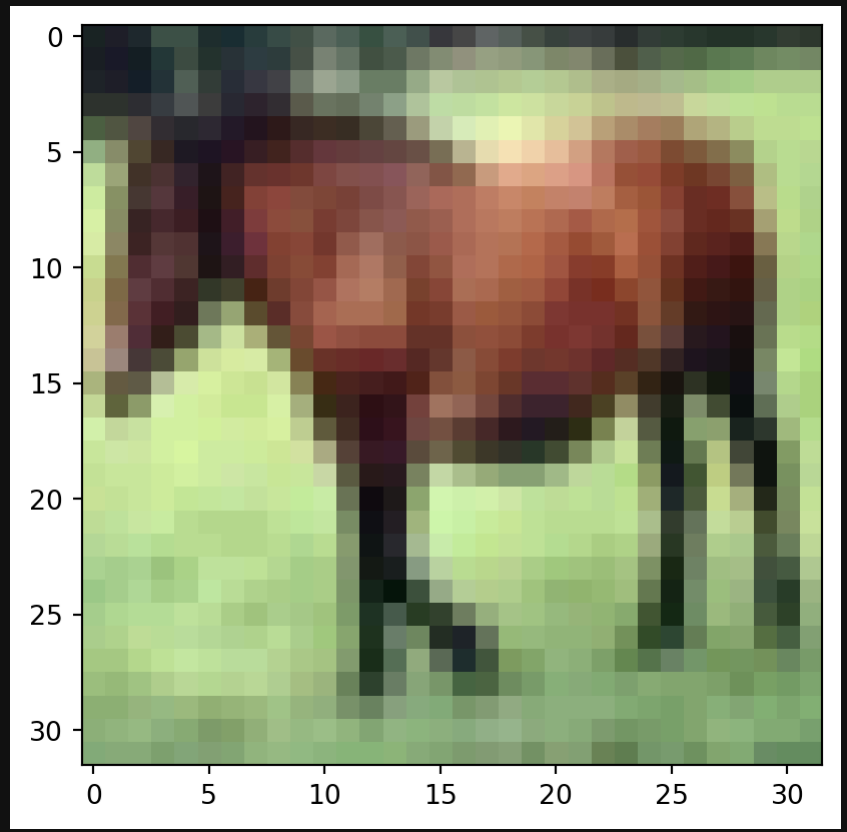
```
Epoch [1000/15000], Loss: 23613.3828
Epoch [2000/15000], Loss: 19056.0820
Epoch [3000/15000], Loss: 15332.7529
Epoch [4000/15000], Loss: 12342.8027
```

```
Epoch [5000/15000], Loss: 10015.9141
Epoch [6000/15000], Loss: 8294.0117
Epoch [7000/15000], Loss: 7116.4990
Epoch [8000/15000], Loss: 6407.3130
Epoch [9000/15000], Loss: 6063.0112
Epoch [10000/15000], Loss: 5949.3794
Epoch [11000/15000], Loss: 5930.7837
Epoch [12000/15000], Loss: 5929.8906
Epoch [13000/15000], Loss: 5929.8848
Epoch [14000/15000], Loss: 5929.8848
```

Datasets

```python
training_data = datasets.CIFAR10(
    root="data",  # path where the images will be stored
    train=True,
    download=True,
    transform=ToTensor()
    )
test_data = datasets.CIFAR10(
    root="data",
    train=False,
    download=True,
    transform=ToTensor()
    )
image, label = training_data[7]
print(f"Label: {training_data.classes[label]}")
print(f"Image size: {image.shape}")
plt.imshow(image.permute(1, 2, 0)) # imshow expects channel order Height x
plt.show()
```

```
Label: horse
Image size: torch.Size([3, 32, 32])
```


0
5
10
15
20
25
30
0
5
10
15
20
25
30

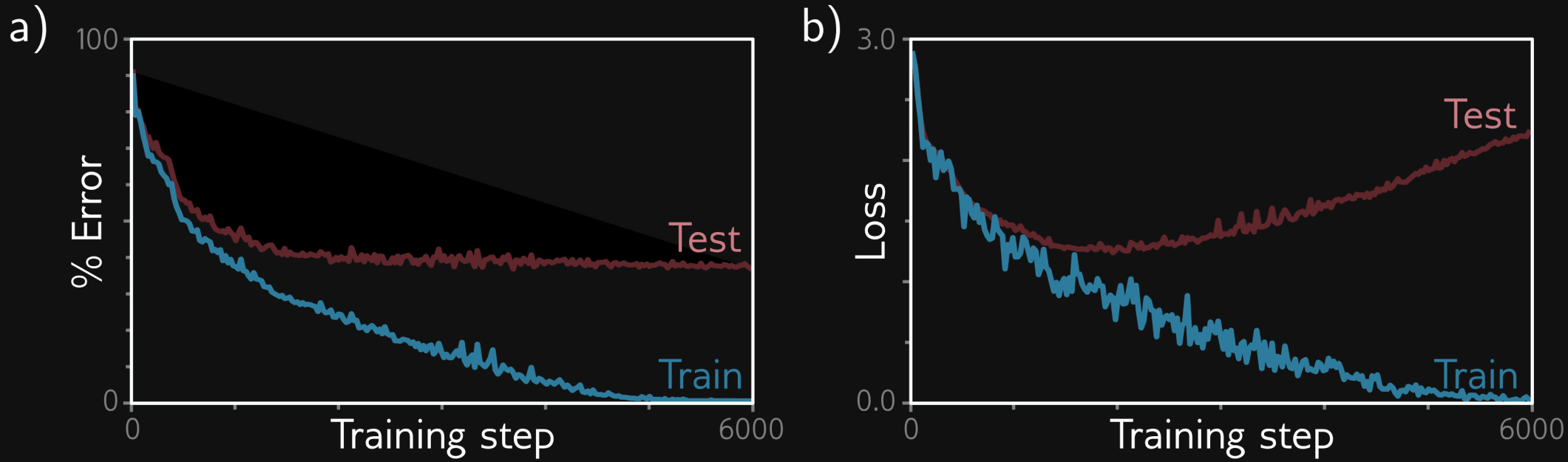
Data Loader

```
# Data Loader for Batching
def seed_worker(worker_id):
  worker_seed = torch.initial_seed() % 2**32
  numpy.random.seed(worker_seed)
  random.seed(worker_seed)
g_seed = torch.Generator()
g_seed.manual_seed(torch.initial_seed() % 2**32)

train_dataloader = DataLoader(training_data, batch_size=64, shuffle=True, r
test_dataloader = DataLoader(test_data,  batch_size=64, shuffle=True, num_w

# Load the next batch
batch_images, batch_labels = next(iter(train_dataloader))
print('Batch size:', batch_images.shape)
plt.imshow(batch_images[0].permute(1, 2, 0))
plt.show()
```

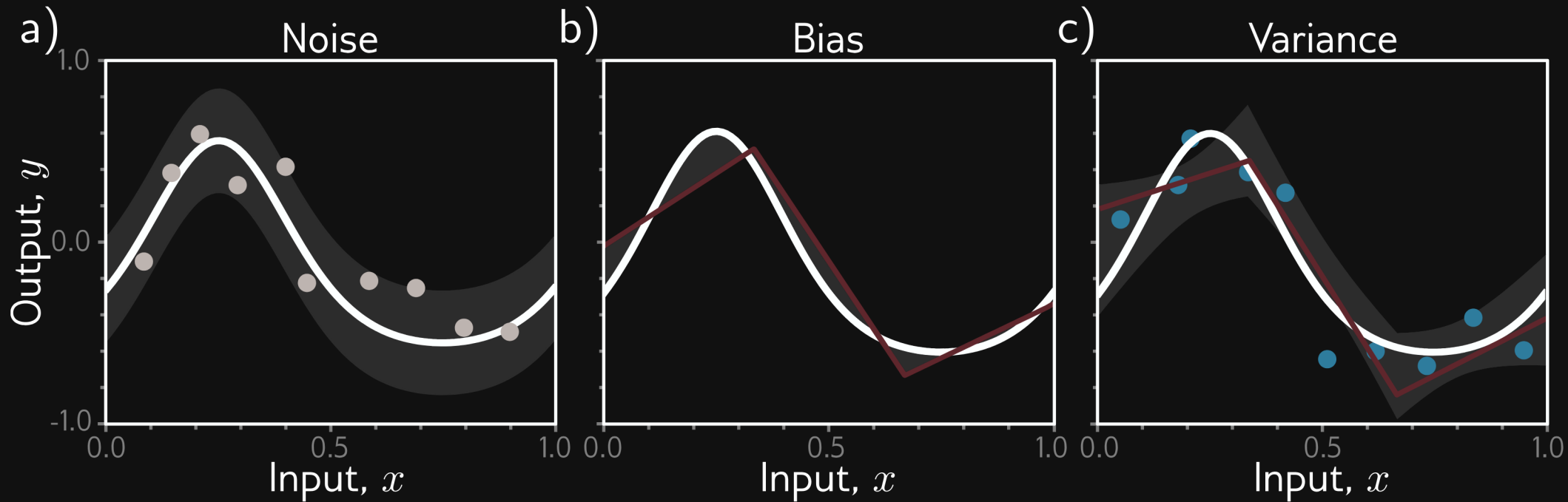
Measuring Performance

Prince (2023, chap. 8)

Training and Test Error



Error Sources



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Error Decomposition

In a linear regression,

$$L[x] = (f[x, \phi] - \mathbb{E}[y|x] + \mathbb{E}[y|x] - y[x])^2$$
$$= (f[x, \phi] - \mathbb{E}[y|x])^2 + 2(f[x, \phi] - \mathbb{E}[y|x])(\mathbb{E}[$$

$y[x]$ and hence L are stochastic, so taking expectations w.r.t. test data y

$$\mathbb{E}_y[L[x]] = (f[x, \phi] - \mathbb{E}[y|x])^2 + 2(f[x, \phi] - \mathbb{E}[y|x]$$
$$= (f[x, \phi] - \mathbb{E}[y|x])^2 + 0 + \sigma^2$$

Taking expectations with respect to training data D

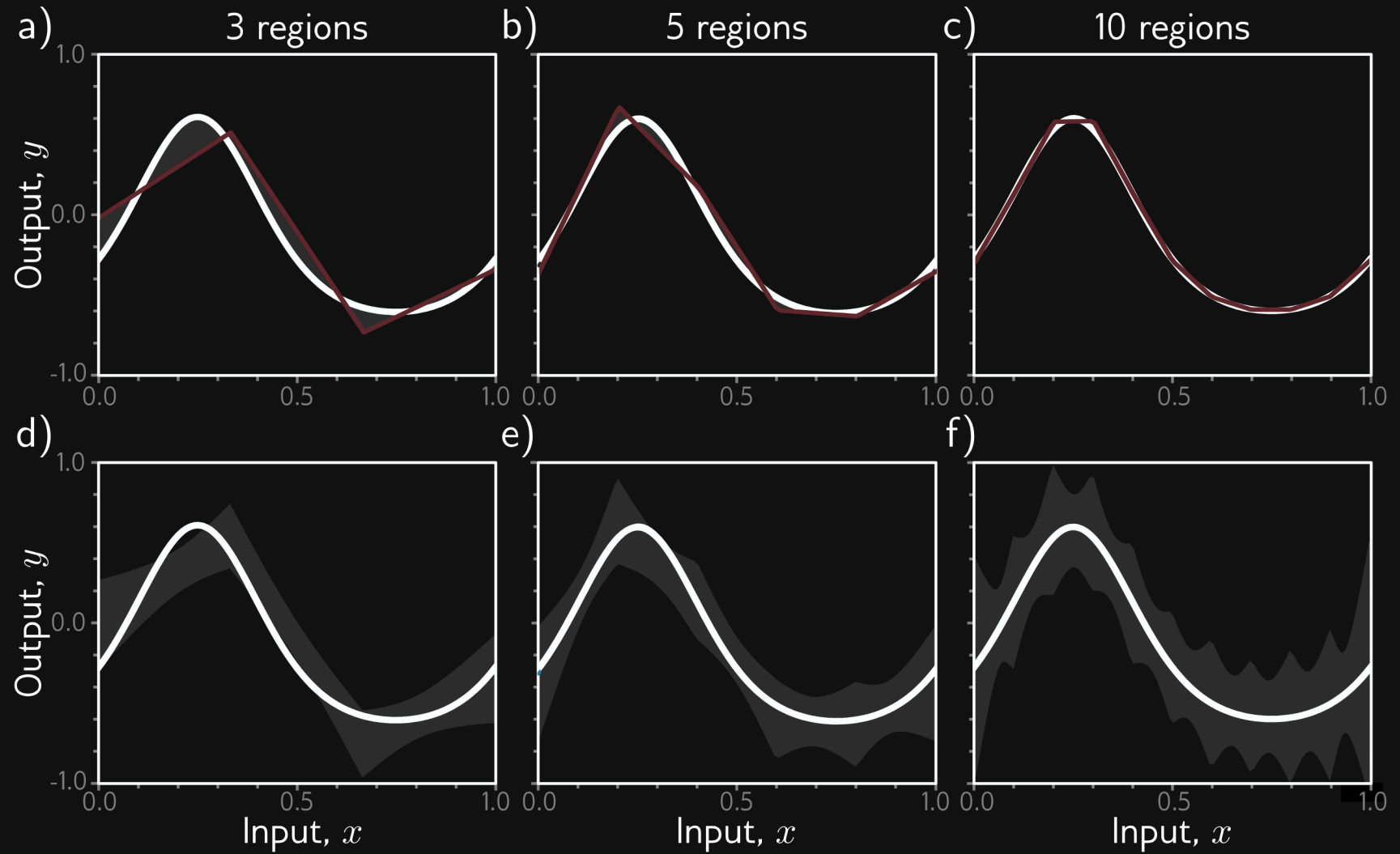
$$\mathbb{E}_D\left[\mathbb{E}_y\left[L[x]\right]\right] = \mathbb{E}_D\left[(f[x,\phi[D]] - \mathbb{E}_D\left[f[x,\phi[D]]\right]\right]$$
$$= \text{Variance} + \text{Bias}^2 + \text{Noise}$$

where

- variance due to sample noise in training data
- bias due to model misspecification
- noise due to inherent uncertainty in $y|x$

More Training Data: Less Variance

Increasing Model Capacity: Less Bias but More Variance



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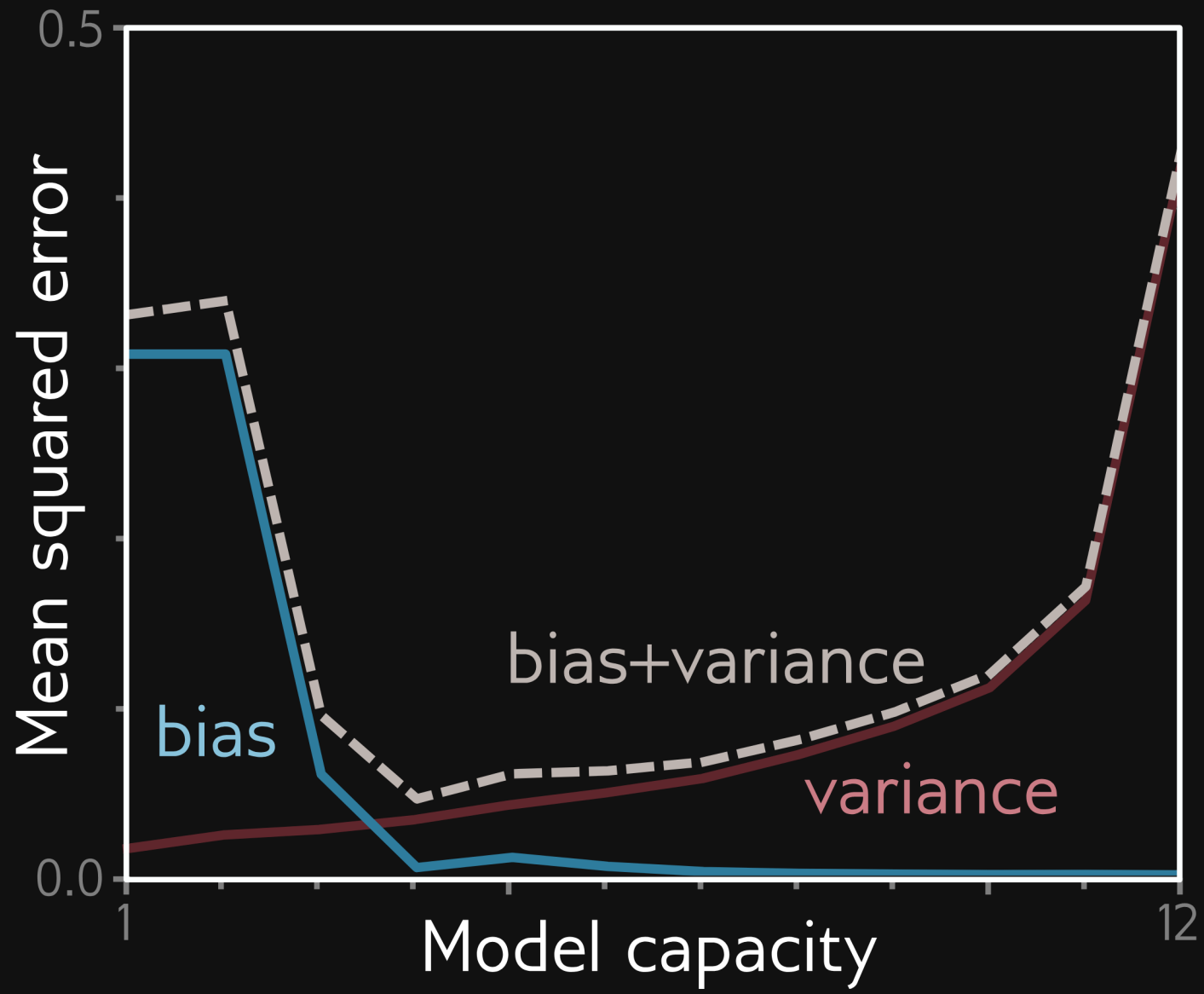
Bias-Variance Tradeoff



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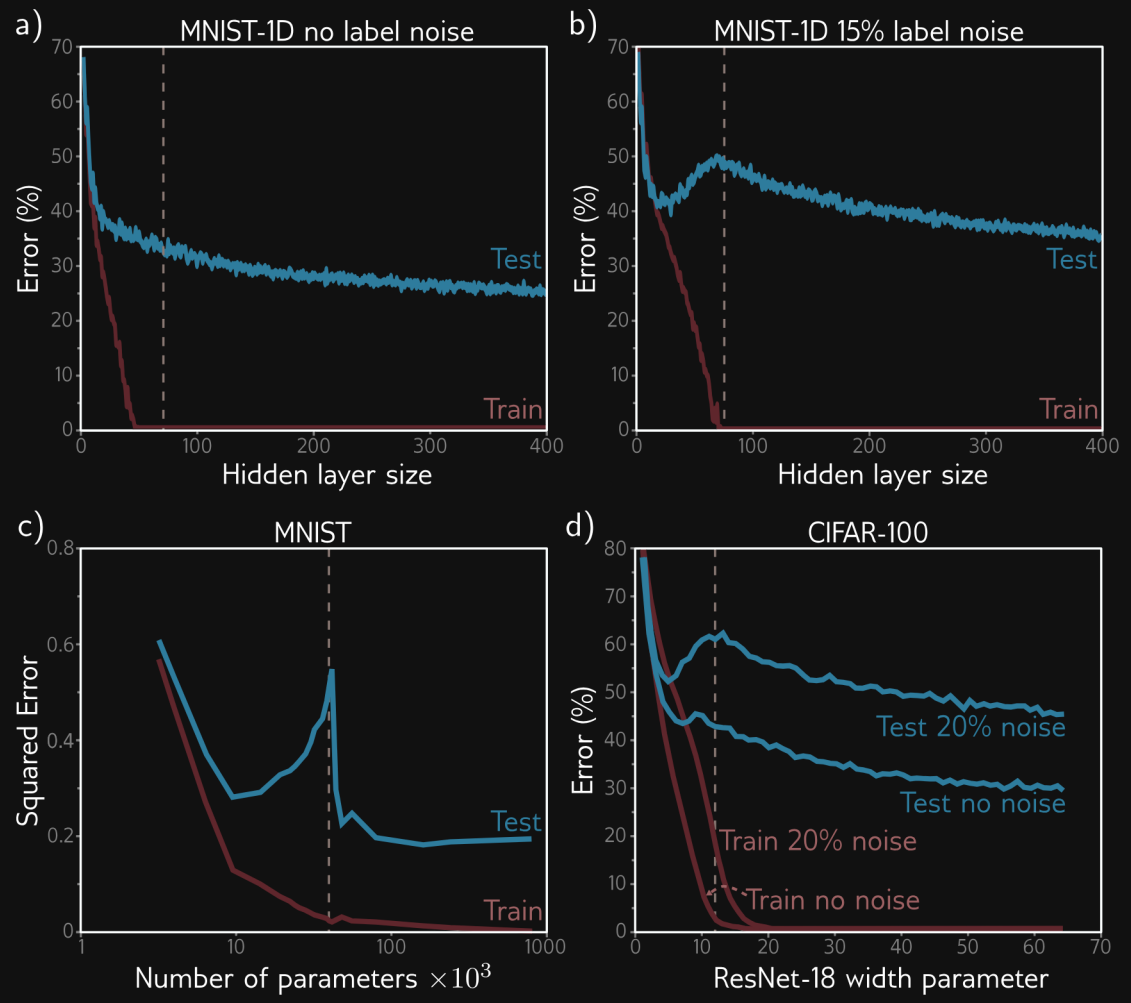
Double Descent (Overparametrization)



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Overparametrization permits (and initialization and/or fitting may encourage) smoother interpolation between training data (implicit regularization), an inductive bias resulting in better generalization.

Cross-Validation

- Learn model parameters on training set
- Choose hyperparameters using validation set
- Evaluate final model on test set

References

Prince, Simon J. D. 2023. *Understanding Deep Learning*. Cambridge, Massachusetts: The MIT Press.