Machine Learning Basics

Vishnu Lokhande

Department of Computer Science and Engineering
Universitpy at Buffalo, SUNY
vishnulo@buffalo.edu

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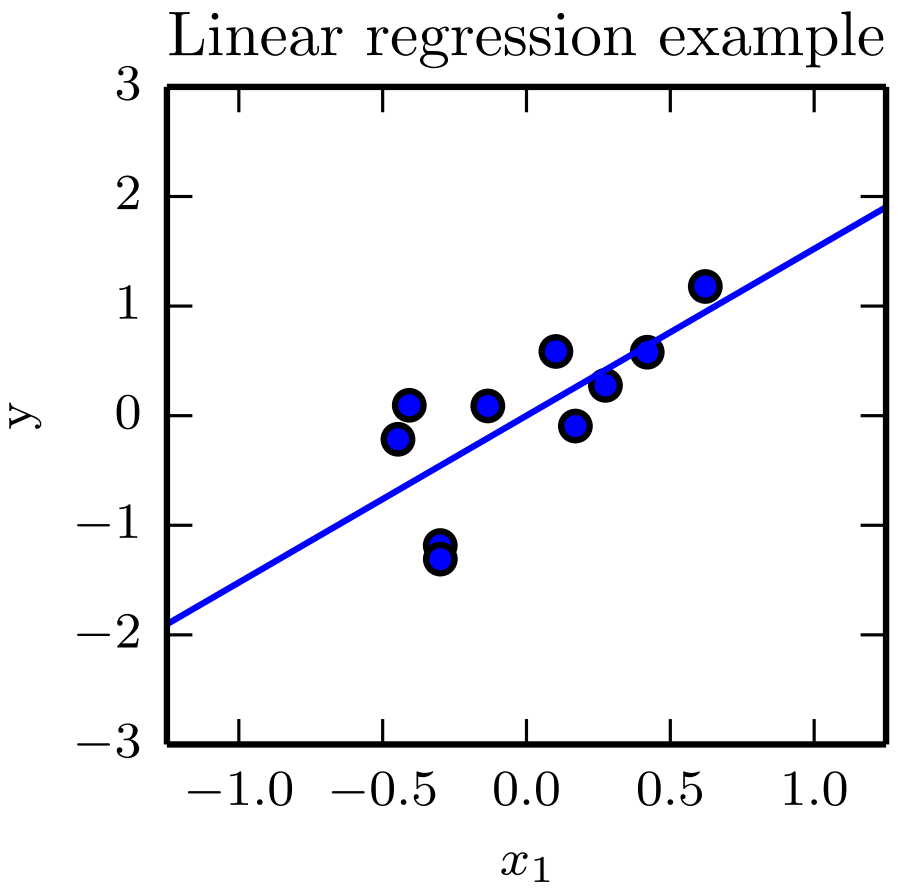
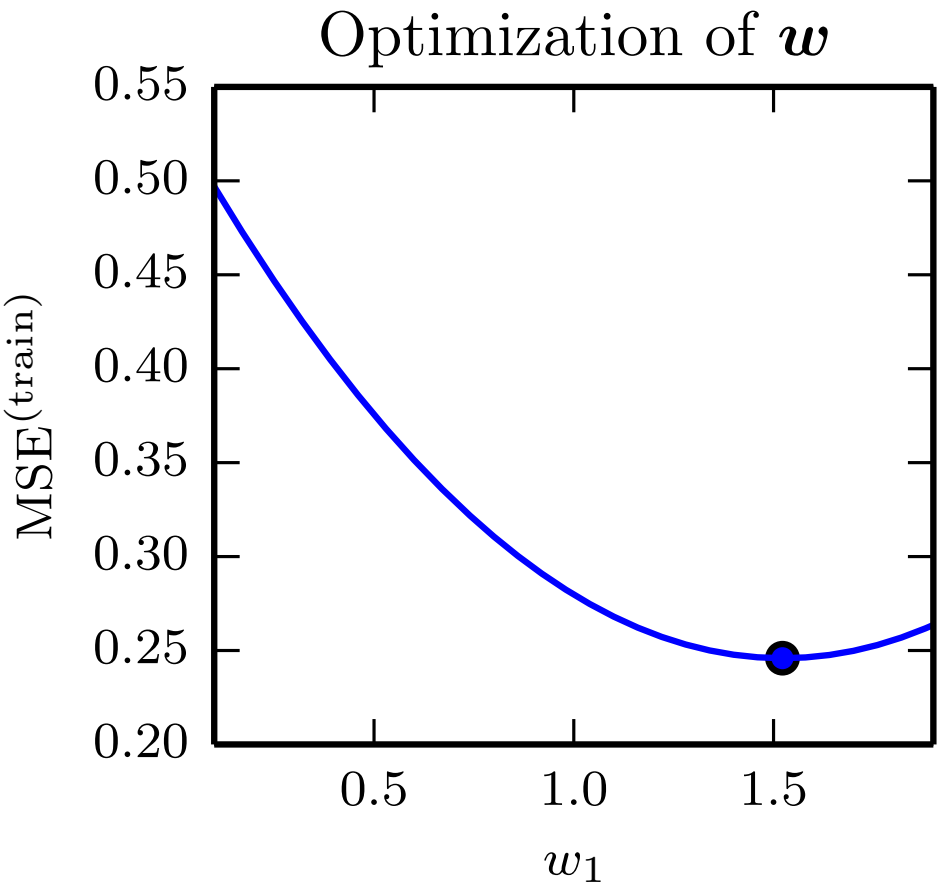
Linear Regression

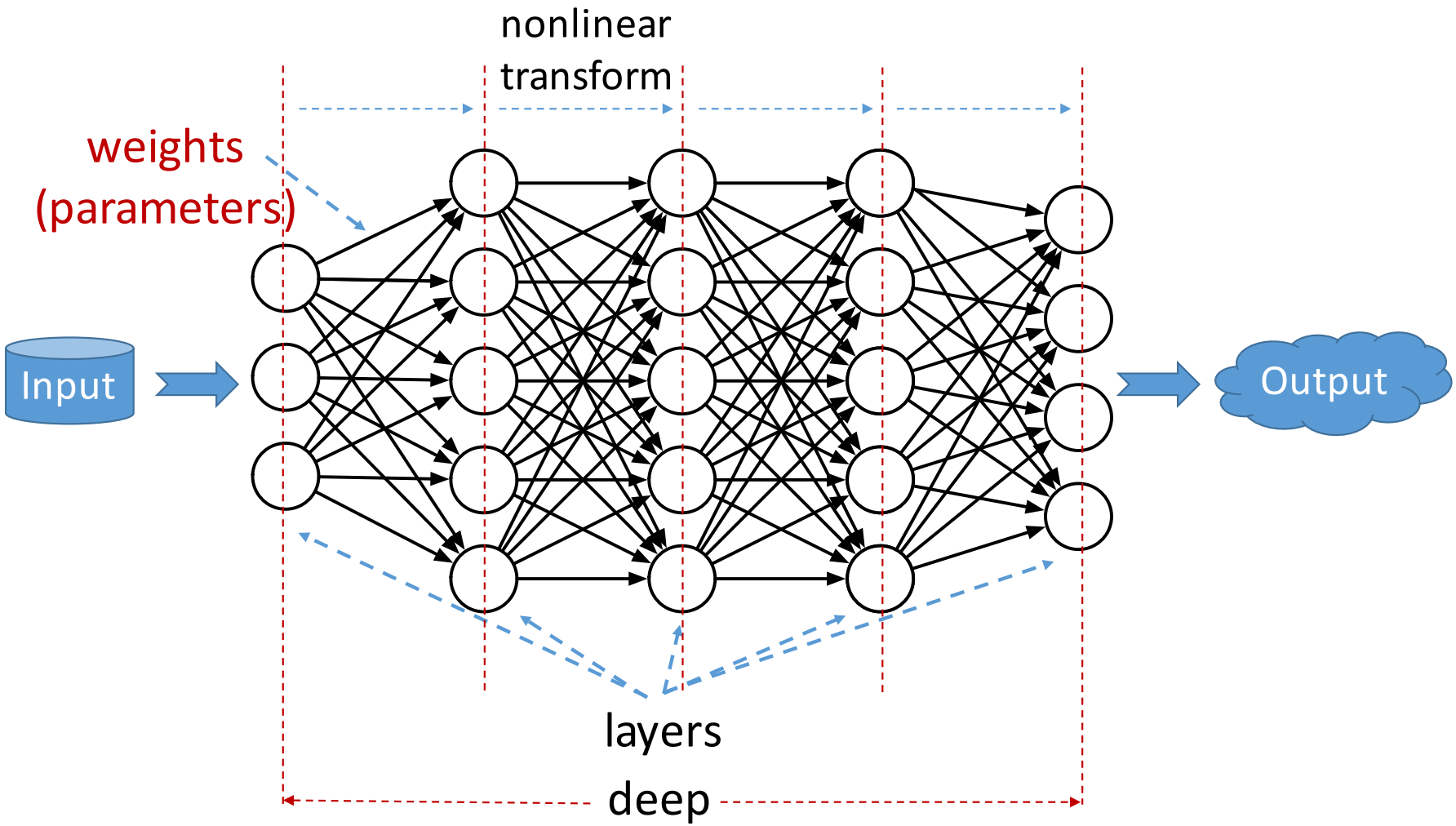
Find a linear model to fit the observed data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$

Objective: $\mathbf{w} = \arg\min_{\mathbf{w}} \sum_{i=1}^{N} \left| \mathbf{w}^T \mathbf{x}_i - \mathbf{y}_i \right|^2$





Deep Neural Networks are Nonlinear Models



Optimization for nonlinear objective functions.

Underfitting and Overfitting in Polynomial Estimation

Model capacity

How flexible a model is.

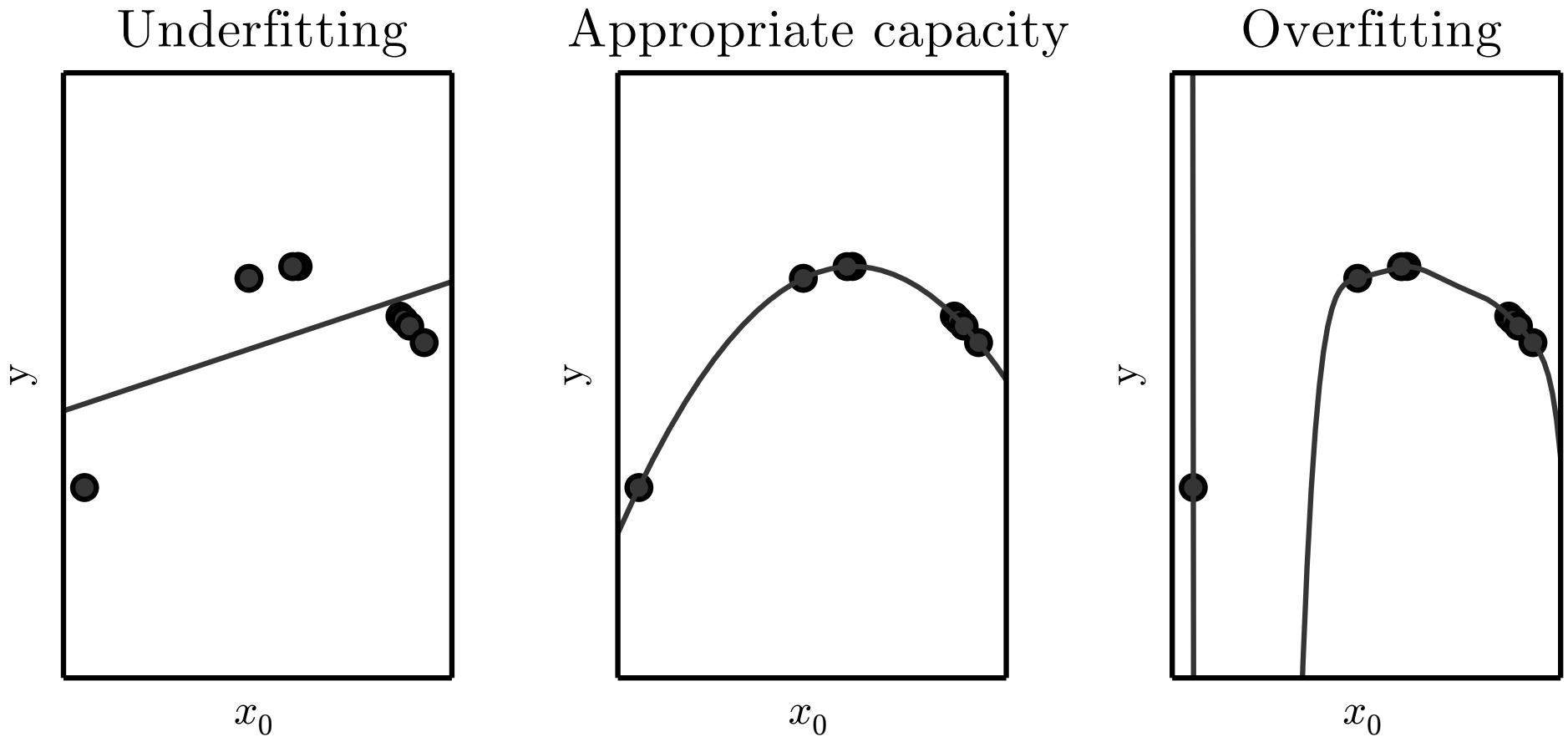


Figure: Left: model too simple (underfitting); Middle: the right model; Right: model too complex (overfitting).

Generalization and Capacity

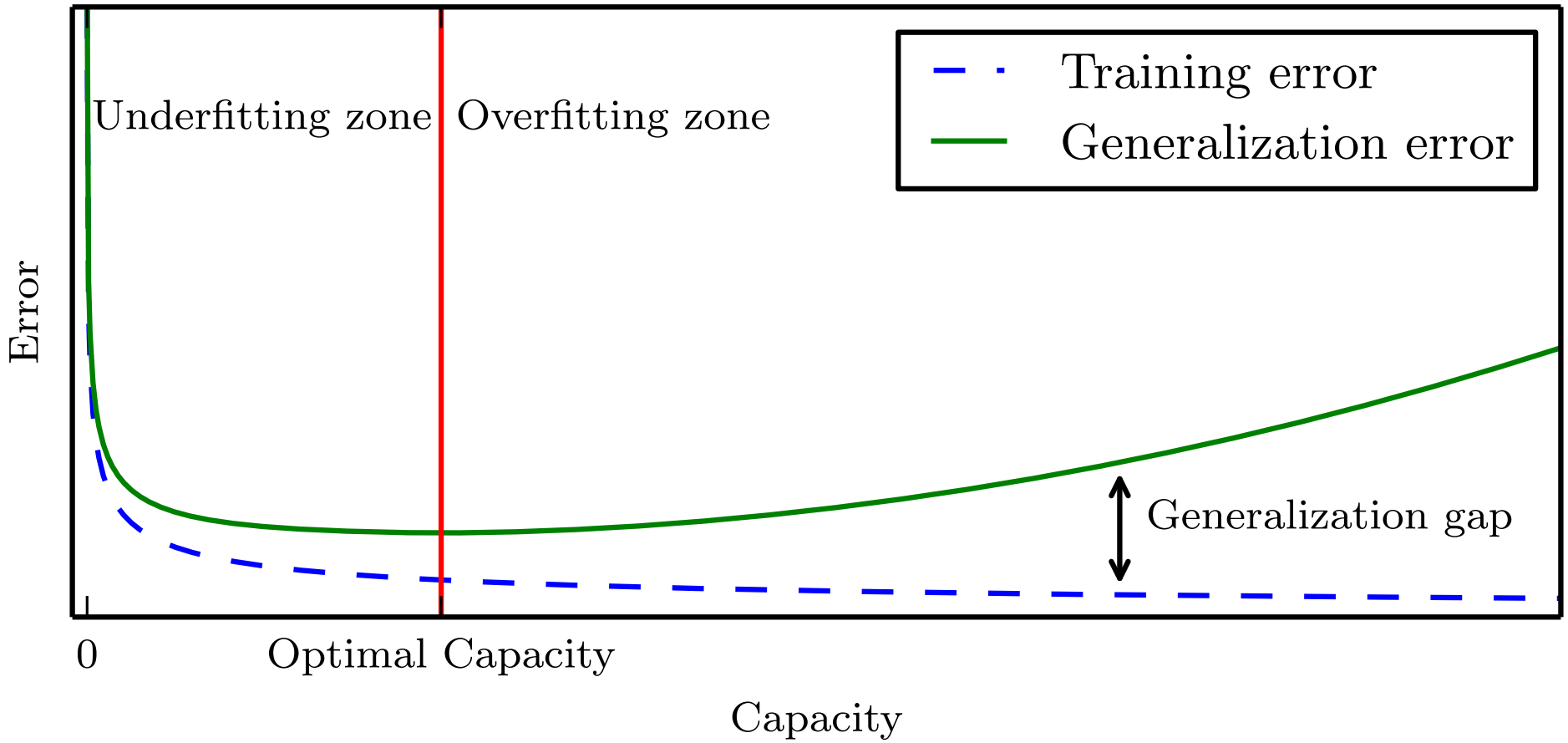


Figure: Training error would decrease with increasing model complexity; whereas the generalization error (applied on unseen data) achieves its lowest error on the right model complexity.

A Different Story for Deep Neural Networks

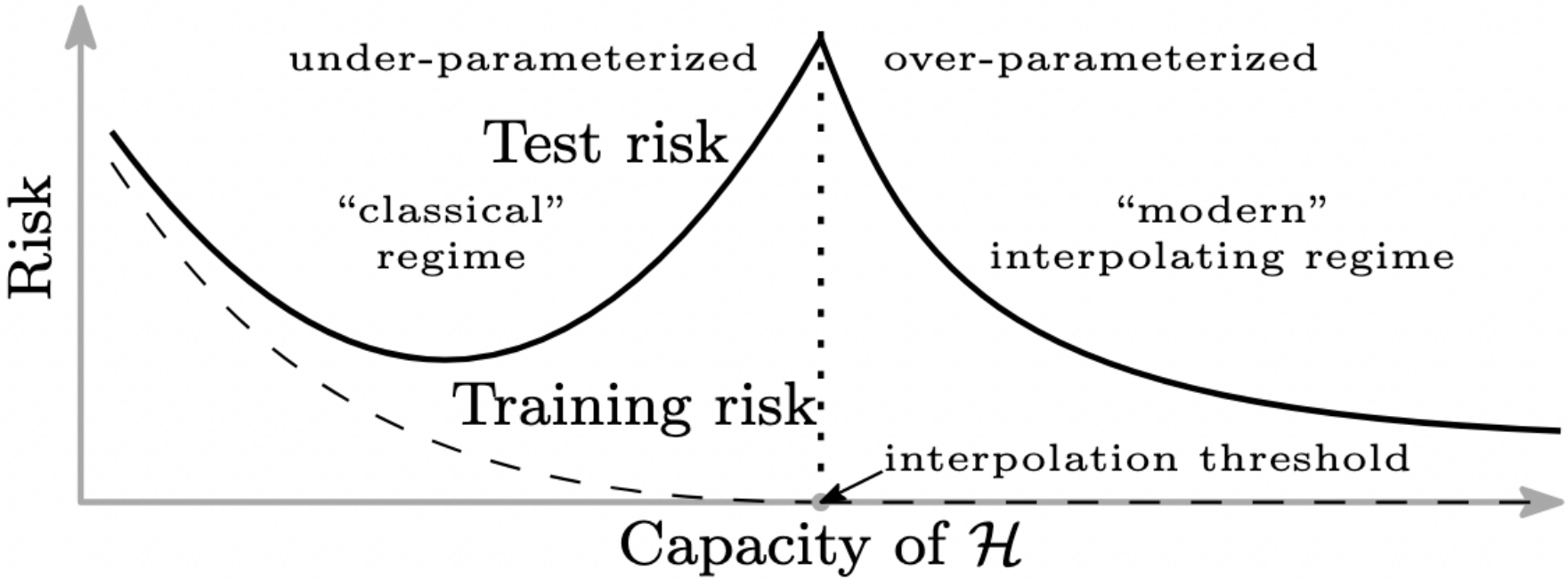
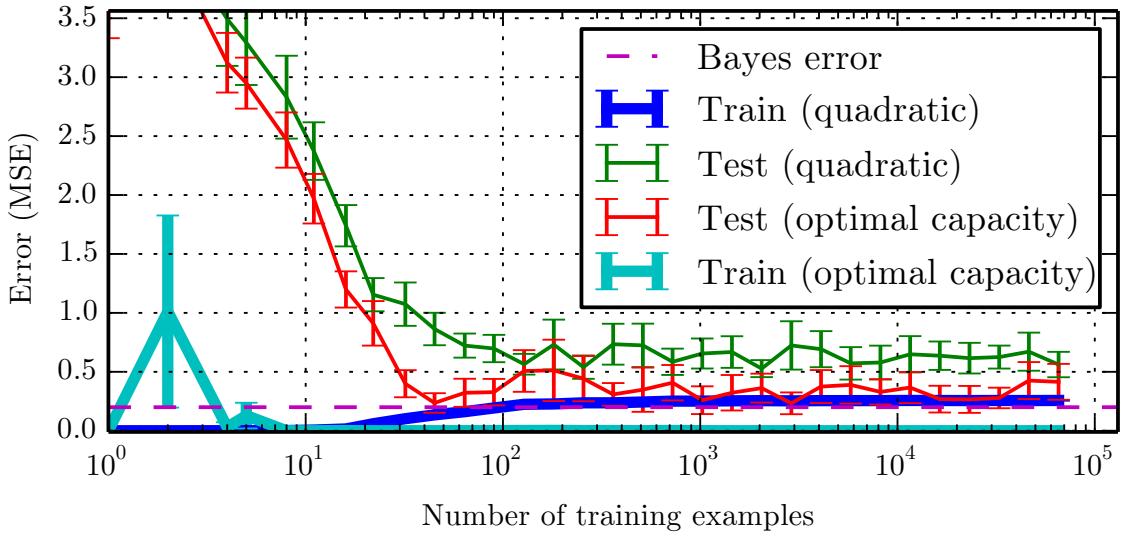
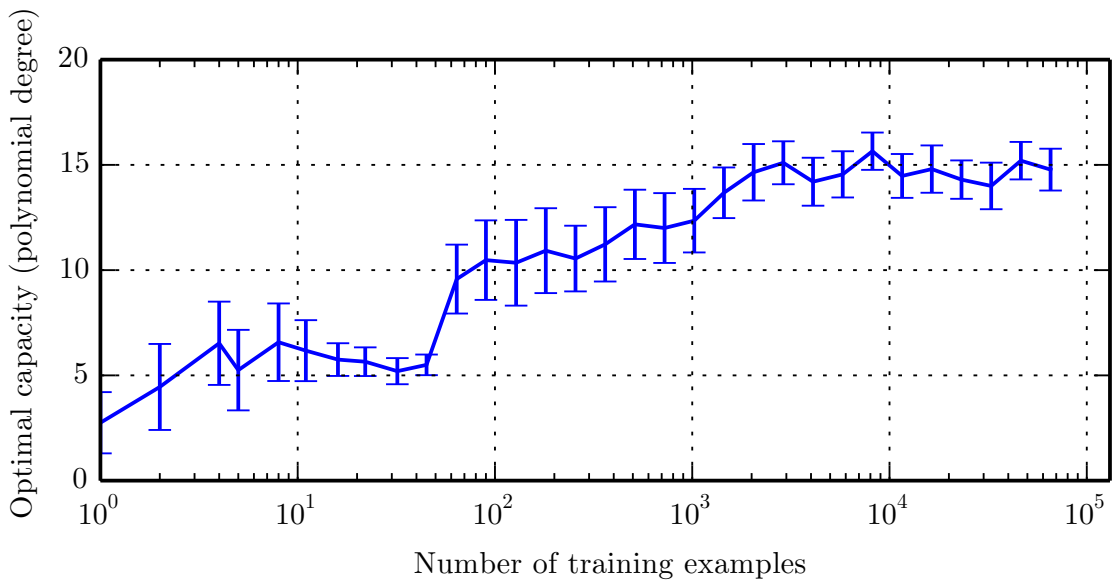


Figure: Double descent in deep neural networks.

Train Set Size VS. Error

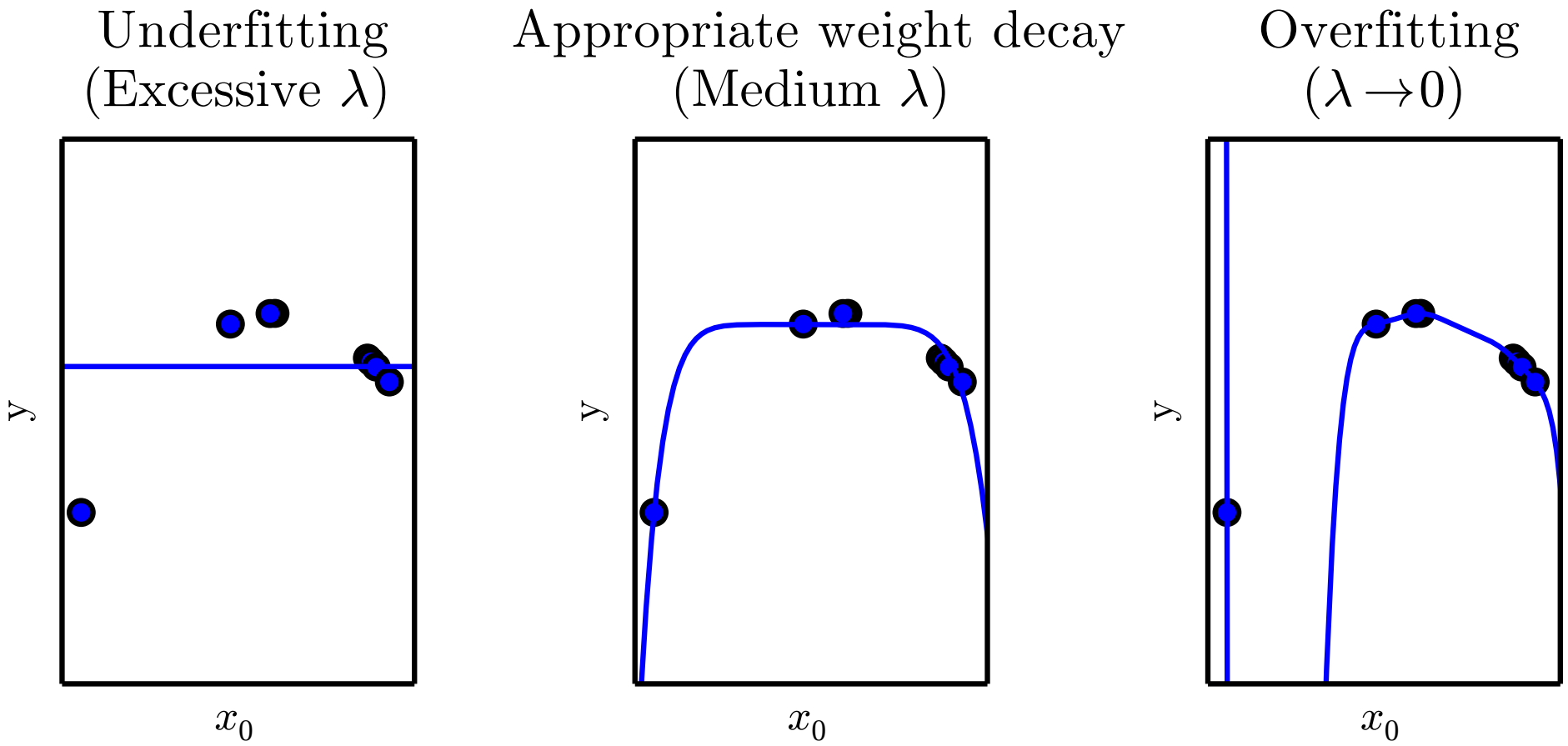
- Bayes error: the best possible error from theory.
- Top: With quadratic capacity: 1) training error increases because more data is harder to training; test error keeps decreases because it gets more information. 2) does not have enough capacity to make the test error lower than the Bayes error.
- Bottom: As the training set size increases, the optimal capacity increases.





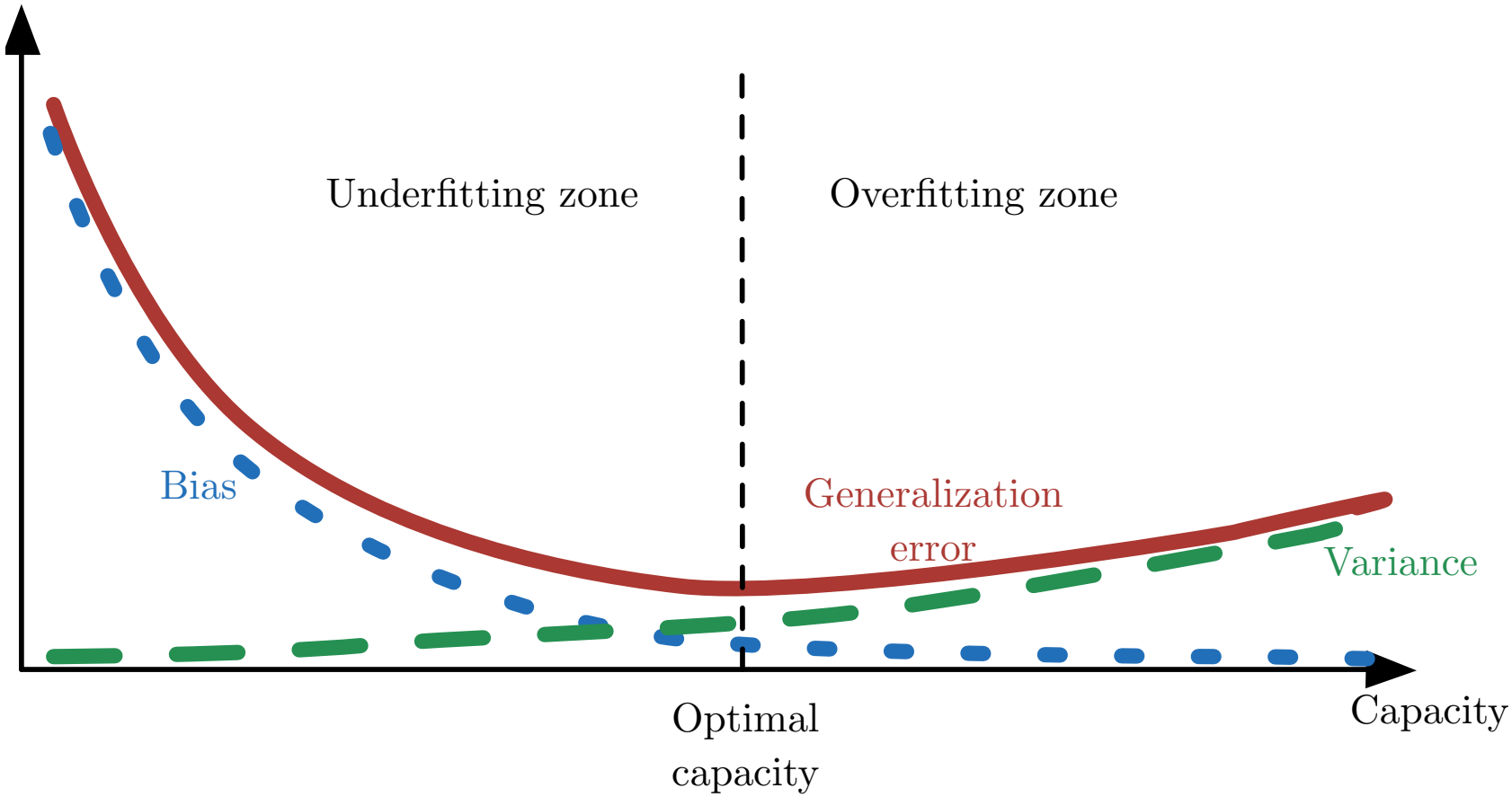
Avoid Overfitting by Weight Decay

$$J(\mathbf{w}) \triangleq \mathrm{MSE}_{\mathrm{train}} + \lambda \mathbf{w}^T \mathbf{w}$$



Bias and Variance

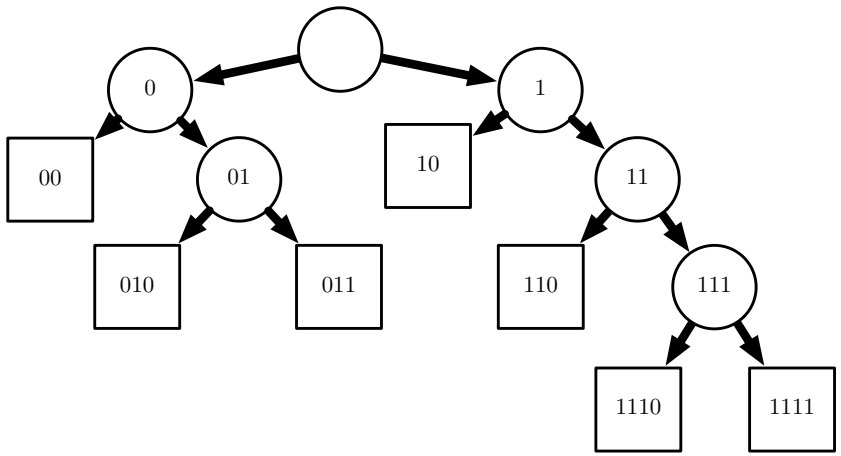
- In the underfitting zone, we usually get high bias (model doesn't fitting the data), but low variance (model behaviors similarly for different test data).
- Opposite in the overfitting zone.

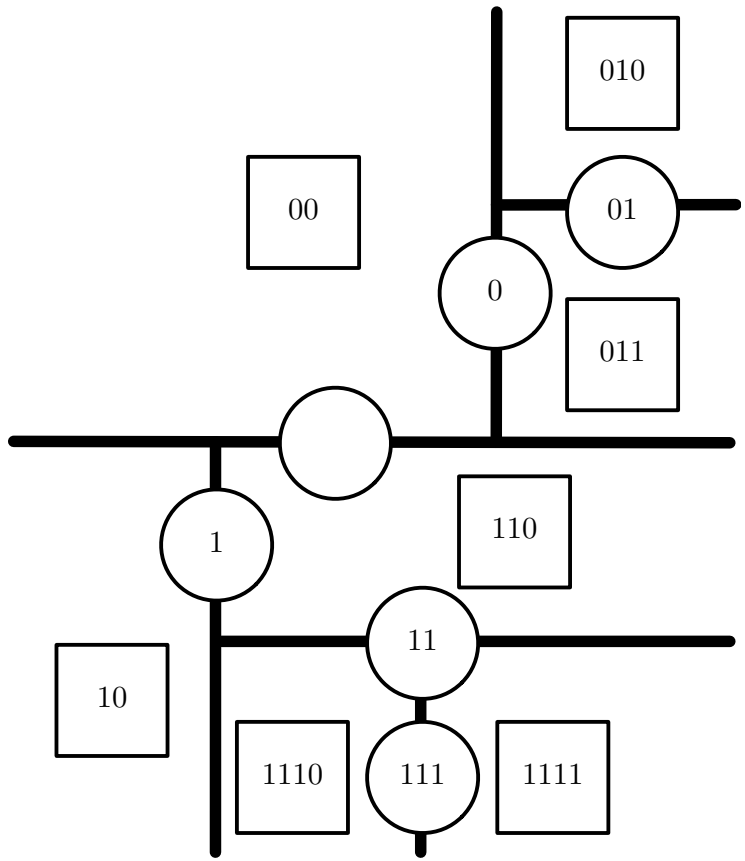


Traditional Nonlinear Models: Decision Tree

In each step, choose a feature, and separate the data according to the chosen feature:

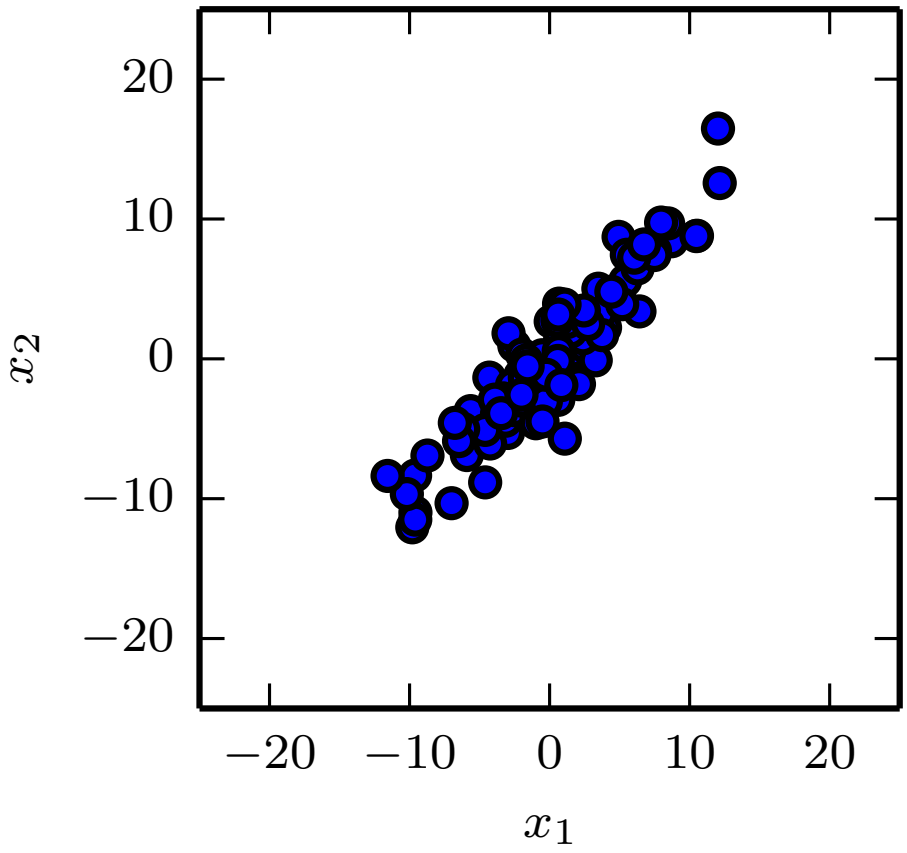
- **Hand-designed features; hard to choose appropriate feature in each step.**

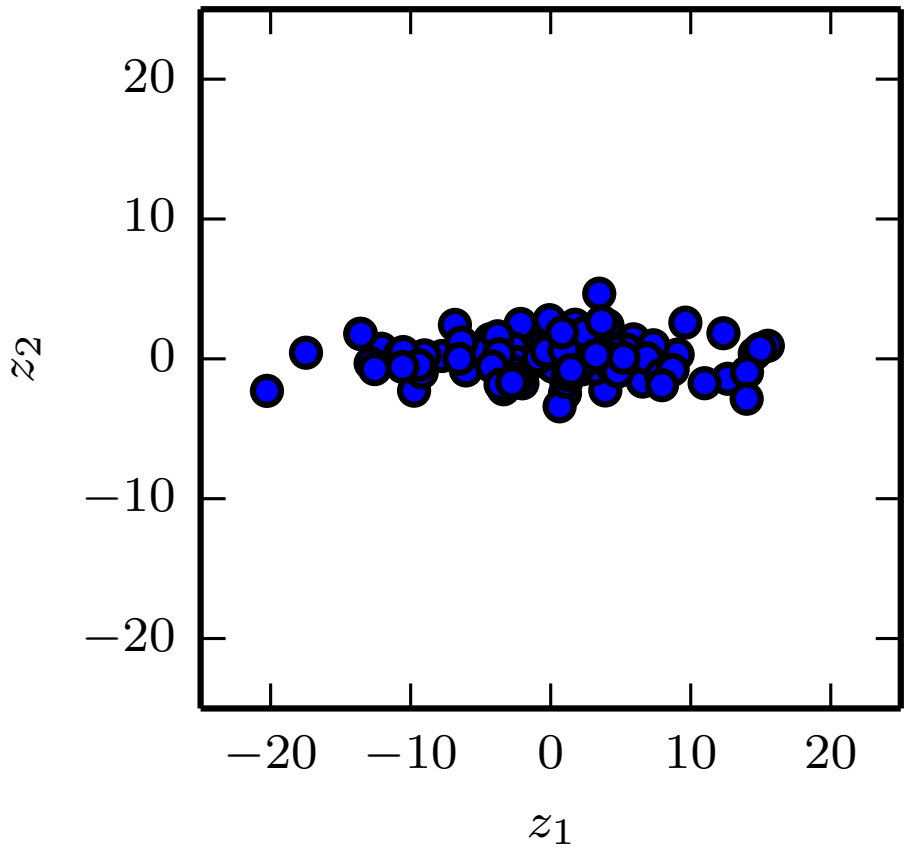




Principal Component Analysis

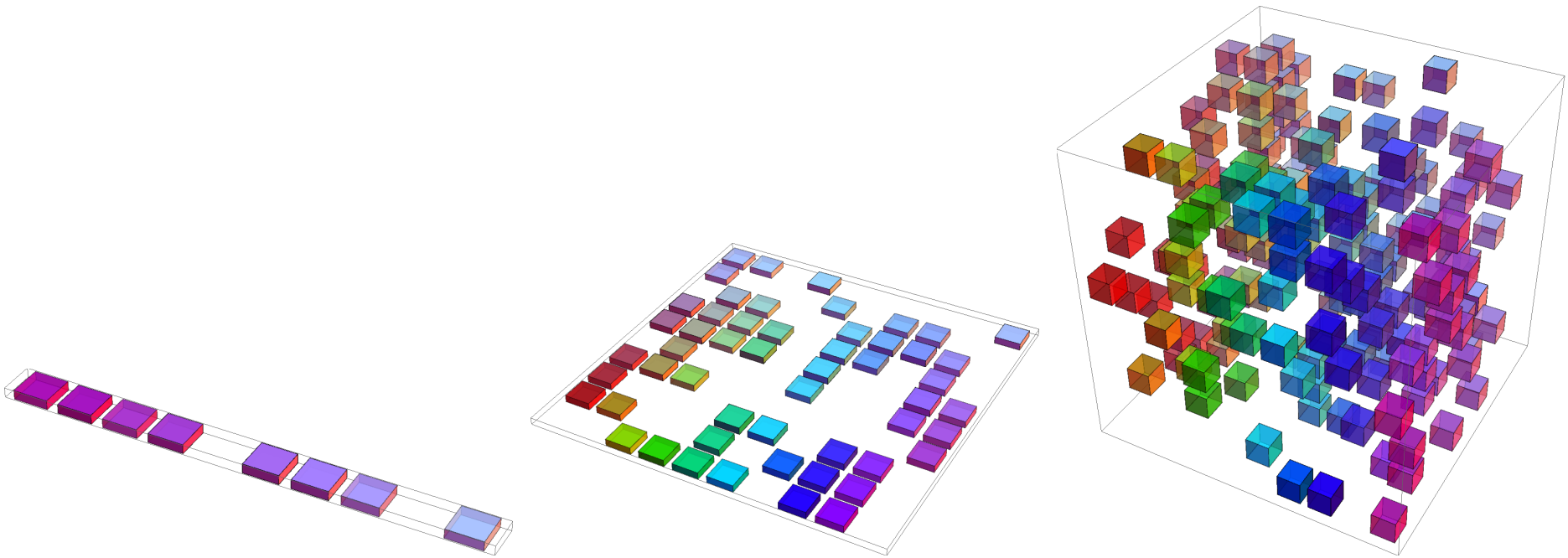
Find a direction that has the most variance (most informative) (right) from the original data (left)





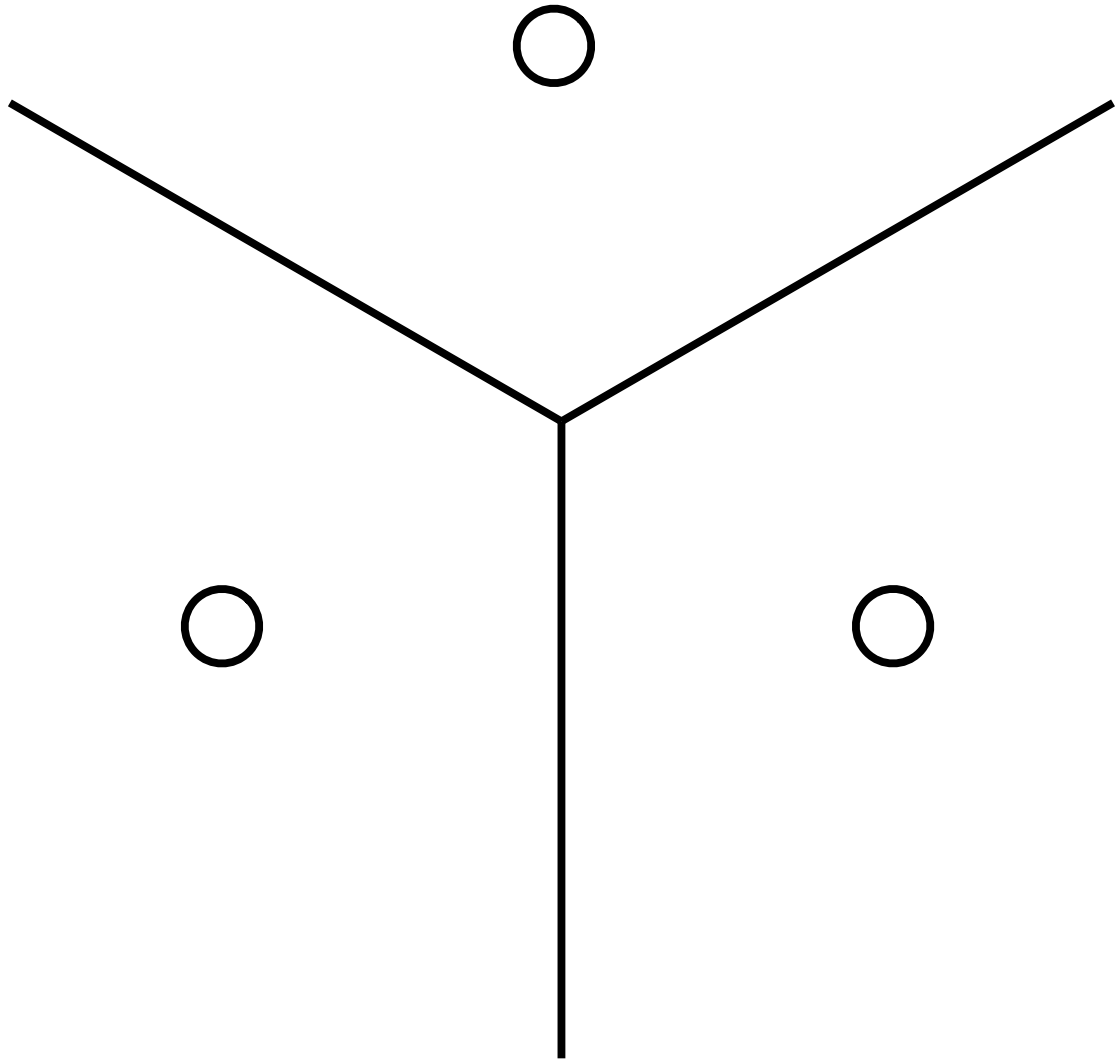
Curse of Dimensionality

- The increase of data can not meet the increase of model complexity:different configurations of model parameters grows exponentially w.r.t. the dimension, thus some regions of the model parameter space does not have data associated.
- Or data is typically sparse in high dimensional space.



Nearest Neighbor

- Classify a test data to the class associated with its nearest train data.



Manifold Learning

- Data typically not flat in the original space.
- They lie in a low-dimensional manifold.
- Fit for deep learning since the manifold is typically nonlinear.