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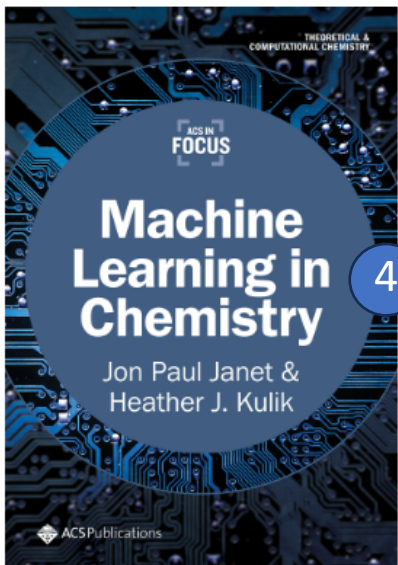
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Machine Learning in Chemistry

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Subjects: Algorithms, Chemical engineering and industrial chemistry, Computational modeling, Machine learning, Neural networks, Theoretical and computational chemistry

Read Time: five to six hours

Collection: Inaugural

Publisher: American Chemical Society



Recent advances in machine learning or artificial intelligence for vision and natural language processing that have enabled the development of new technologies such as personal assistants or self-driving cars have brought machine learning and artificial intelligence to the forefront of popular culture. The accumulation of these algorithmic advances along with the increasing availability of large data sets and readily available high performance computing has played an important role in bringing machine learning applications to such a wide range of disciplines. Given the emphasis in the chemical sciences on the relationship between structure and function, whether in biochemistry or in materials chemistry, adoption of machine learning by chemists. *Machine Learning in Chemistry* focuses on the following to launch your understanding of this highly relevant topic:

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Preface

1. Advancing Research through Machine Learning

2. Supervised Machine Learning for the Chemical Sciences

3. Linear Models, Kernels, and Trees

4. Representations of Atomistic Systems

5. Neural Networks and Learned Representations

6. Applying Machine Learning Models in Chemistry

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Jon Paul Janet is a scientist with expertise in molecular machine learning. He is currently working on early stage drug discovery and previously developed machine-learning augmented virtual design strategies for inorganic complexes. He received a Ph.D. in

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Jon Paul Janet & Heather J. Kulik

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Abstract
Recent advances in machine learning or artificial intelligence for vision and natural language processing

CHAPTER 1

Advancing Machine Learning in Chemistry

- 1.1 Overview
- 1.2 Machine Learning Techniques
- 1.3 Machine Learning in Materials Chemistry
 - 1.3.1 Revealing Patterns in Chemical Data Applied to a variety of problems in chemistry, and novel applications
 - 1.3.2 Overcoming the Limits of Simple Models and Human Experience
 - 1.3.3 Accelerating Computations and Analysis to Enable Rapid Discovery in Challenging Materials Spaces

1.1 OVERVIEW

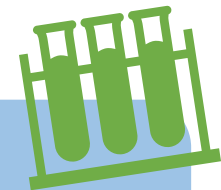
Interest in merging machine learning with traditional scientific inquiry has surged in recent years among researchers in the physical sciences. In laboratories across the world, scientists are identifying ways to incorporate machine learning into their everyday research. In both experimental and theoretical chemistry, recent applications have included the development of reactive force fields trained on first-principles data;^{1,2} rapid property prediction models for materials discovery;³⁻⁶ and the prediction, design, and improvement of catalysts^{7,8} or chemical reaction yields.⁹ “Machine learning” is a broad term for statistical algorithms that build prediction or decision models based on inferences from available data without explicitly coded instructions or a predefined parametric form.

Machine learning in chemistry is not new (Figure 1.1).¹⁰⁻¹⁵ A similar surge in interest in applying machine learning (e.g., **artificial neural networks**) occurred in the late 1980s to mid-1990s.¹² The earliest applications of data science techniques to chemical problems included the development of feedback-trained expert or decision-based systems¹⁰ and dimensionality reduction and pattern recognition using chemical data sets.¹⁶⁻¹⁸ By the 1990s, the computer science community had demonstrated that nonlinear models, such as neural networks, could model any input-output mapping¹⁹ (e.g., with sufficient **hidden layers**); this had not previously been thought possible in the early stages of applying simple acceptance models that

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