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From Data to knowledge by domain knowledge and machine learning

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The extremely fast progress of data science, artificial intelligence, and machine learning accelerates the development of materials informatics. Material (or mechanics) feature space is usually of high-dimensions, including chemical composition, phase and crystal structures, defect types and configurations, material process conditions, testing conditions, service environment, etc. On the other hand, available material (or mechanics) data are typically sparsely distributed, not big at all. How to machine learn small data and gain knowledge is a great challenge in materials informatics (or mechnoinformatics). The present presentation emphases the joint effort of domain knowledge and machine learning that spends up the learning process from data to knowledge. The academic argument on the size-dependent strength of concrete is taken here as an example to illustrate the significance of the joint effort, where the data is so small without the failure probability information for each given sample size. Integrating Weibull distribution into expectation maximization algorithm allows one to determine the failure probability density distribution by using the entire data for all sample sizes. The machine learning gives the result that with the survival probability of 99%, no failure will occur if the max bending stress is 6.2 MPa for the smallest sample size with the beam height of W=40mm, 5.6 MPa for W=93mm, 5.1 MPa for W=215mm, and 4.6 MPa for the biggest sample size with W=500mm. The result indicates that the smaller the sample size is, the stronger the concrete samples will be. The machine learning also provides the strength Weibull distribution, in which the stress component does not change with sample size, whereas the reference stress (strength) varies with sample size.

*The ML is conducted by Mr. Jiahao Wang and Mr. Junnan Jia.