

Glossary

Artificial intelligence is the ability of a machine to perform a task that would usually require the natural intelligence displayed by humans or animals.

Axiom is a statement that is taken to be true, to serve as a premise or starting point for further reasoning and arguments.

Bioactivity is an effect on, interaction with or response from a living tissue or cell.

Biocompatibility is the ability of a material to perform its function with an appropriate host response without causing any undesirable local and systemic effects.

Biodegradation is the mechanical, physical and chemical modification of a material by a biological environment and associated cells to break it down to its monomeric form.

Biological assay is an analytical method to determine the concentration or potency of a substance by its effect on living animals or plants (in vivo), or on living cells or tissues (in vitro).

Biological environments are cellular and physical surroundings of an organism, includes the factors that have an influence in their survival, development, and evolution.

Biological molecules is a term for molecules present in organisms that are essential for one or more biological processes, such as cell division, morphogenesis, or development.

Black-box model is a system which can be viewed in terms of its inputs and outputs (or transfer characteristics), without any knowledge of its internal workings.

Cell phenotype is the set of observable characteristics or traits of a cell.

Chemical design space is the property space spanned by all possible molecules and chemical compounds adhering to a given set of construction principles and boundary conditions.

Chemical diversity is the variety of chemical compounds present in an environment.

Chemical resolution is the degree of detail that can be achieved in measuring differences between molecules in an environment.

Cross-validation is a model validation technique for assessing how the results of a statistical analysis will generalize to an independent data set.

Descriptors are words or features that serve to describe or identify something.

Design of Experiments is an organized method to study the relationship between multiple input variables and key output variables.

Empirical statistical (method) is used to describe and summarize empirical data in a convenient way.

False negative is an error where the test result incorrectly indicates the absence of a condition when it is present. Example: An individual is diagnosed negative for diabetes when they have the disease.

False positive is an error where the test result incorrectly indicates the presence of a condition (such as a disease when the disease is not present).

Finite element method is a widely used method for numerically solving differential equations arising in engineering and mathematical modelling.

Full factorial design is an experiment design where all the levels of all the factors are combined with one another. For example, if there are 2 factors, and each factor has 3 levels, then all possible combinations to perform the experiment is $2^3 = 8$.

Genetic methods (materials design) are iterative approaches to materials design where materials are repeatedly synthesized, tested and then slightly modified in order to optimize the structure of a material for a particular performance criterion.

Hidden layer is a layer in between input and output layers in a neural network, where artificial neurons take in a set of weighted inputs and produce an output through an activation function.

Homopolymer is a chain of chemically linked molecules that are identical to each other.

In vitro means studies performed with microorganisms, cells, or biological molecules outside their normal biological context.

In vivo means studies in which the effects of various biological entities are tested on whole, living organisms or cells, usually animals, including humans, and plants.

Input data is the first set of data that a neural network uses to make a prediction.

Kernel methods are a class of algorithms for pattern analysis with the general task to find and study general types of relations (for example clusters, rankings, principal components, correlations, classifications) in datasets.

Locally optimal properties are conditions where small increases or decreases to a material's properties do not improve the material's performance even though the conditions do not achieve the optimal performance.

Machine learning methods are approaches where a computer is able to train itself to perform a task, including supervised/unsupervised learning and reinforcement learning.

Material stiffness is the measure of a material's ability to resist deformation when acted on by an external force.

Materials design space refers to all the possible different material formulations.

Mechanical interaction is the capacity of an object to influence the motion of another object.

Model components are the variables associated with the subject of a model and the processes that link the variables together.

Molecular fingerprinting is a method of encoding the structure of a molecule in which a series of binary digits (bits) represents the presence or absence of particular substructures in the molecule.

Nodes are computational units that have one or more input connections. Input from the data is combined with a set of coefficients, that either increase or diminish it, thereby assigning significance to inputs according to the task the algorithm is trying to learn.

Non-fouling refers to the ability to resist the adsorption of biomolecules, such as proteins, or adhesion of cells.

Nonlinear is a system in which the change of the output is not linearly proportional to the change of the input.

Ontologies are detailed formalizations of a certain area of knowledge using a conceptual scheme. It consists of a data structure containing all relevant classes of objects and rules (theorems, restrictions) adopted in this area.

Output layers are the last layers that produce the final computational results in neural networks.

Overfit the production of an analysis that corresponds too closely or exactly to a particular set of data, and may therefore fail to fit additional data or predict future observations reliably

Partial factorial design consists of a carefully chosen subset of the experimental runs of a full factorial design.

Physicochemical involves both physical and chemical properties of a substance.

Predictivity is a condition when it is possible to accurately forecast future states of the system.

Provenance is a detailed record of model organism origin and history, to preserve its scientific significance.

Quantitative structure-property relationships are relationships between chemical structure and biological activity or chemical property of a biomaterial.

Readout is a visual record of the experiment.

Regenerative medicine deals with the process of replacing, engineering or regenerating human or animal cells, tissues or organs to restore or establish normal function.

Robustness is the property of a model when its outputs and forecasts are consistently accurate.

Self-oxidation is the property of a substance to react with itself in the presence of oxygen.

Structure-function relationship is the reliance relationship between the physical and chemical properties of a material on its functional properties.

Synergistic effects are interactions or cooperation giving rise to a whole that is greater than the simple sum of its parts.

Synthetic polymers are human-made substances or materials consisting of very large molecules and composed of repeating units.

Test set is a data set used to provide an unbiased evaluation of a final model fit on the training data set. The test set is not used to create the model.

Tissue engineering is the design and fabrication of living replacement devices for surgical reconstruction and transplantation.

Topography is the architectural landscape of the surface of a (bio)material.

Total data set is a collection of analytical results for all required variables.

Training set is the data initially used to create a computational model.

Transfer function is the ratio of the output of a system to the input of a system.

White-box modelling is an abstract representation of a complex system in terms of equations or rules and a description of the region (spatially and/or temporally) on which these rules are valid.

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