MSc Future Power Networks Smart Grid Technology (ELEC97077) Machine Learning and Data Science for Power Systems

A Closer Look

Dr. Wangkun Xu
wangkun.xu18@imperial.ac.uk

Department of EEE, Imperial College London

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Outline I

Outline II

Outline

Overview I

- 4-5 hour lectures to cover the **BASIC** idea of machine learning, deep learning, and foundation model.
- Coursework, including both numerical and simulation questions.
- Maybe an extra hour tutorial on coursework.
- About myself:
  - Wangkun Xu, Research Associate in the department.
  - Obtained my PhD in 2024 at Imperial.
  - Main research direction on machine learning for robust and secure power system operations.
  - Website: `https://xuwkk.github.io/wangkun_xu/`.
  - GitHub: `https://github.com/xuwkk`.
  - Blog: `https://xuwkk.github.io/blog/`.
- Contact me via email or MS Teams regarding on the course or any inquiry. Please share with me any typo in the slides and suggestions of this course!

Outline

Machine Learning: Why and What I

You probably know that the new trend of large penetration of **renewable energy** challenges the old model-based control room techniques.

Machine Learning: Why and What II

New challenge one: The grid with power electronics becomes a **black box** to the system operators. The inverters can cause new stability issues in the grid.

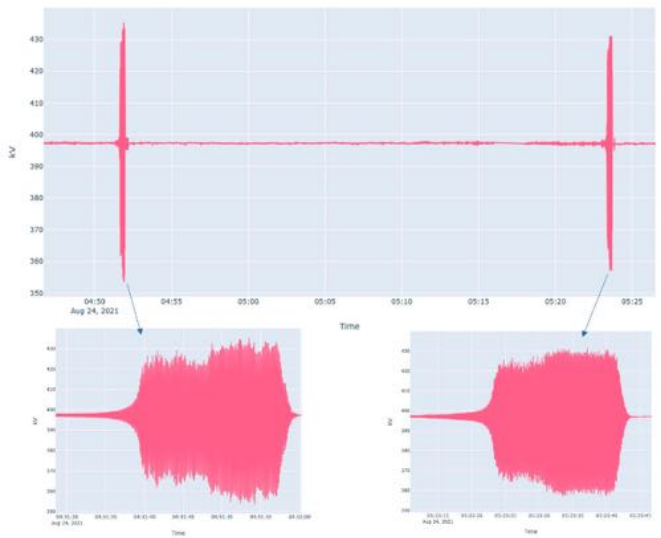


Figure: Sub-synchronous voltage oscillations (8Hz) recorded in GB transmission system, North Scotland, in 2021 [Source: NESO Report on Sub-synchronous oscillations in GB].

Machine Learning: Why and What III

New challenge two: Compared to traditional energy resources, renewable energy is more difficult to manage.

New opportunity: We are entering the era of **big data**. As the advances of **digitalization** in power system, more and more data from the measurement unit, such as remote terminal units (RTUs), phasor measurement units (PMUs), and smart meters, are readily available. But how to extract useful information from the data is one thing we need to consider.

Machine Learning: Why and What IV

This requires automated data analysis methods, which is what *machine learning* (ML) provides.

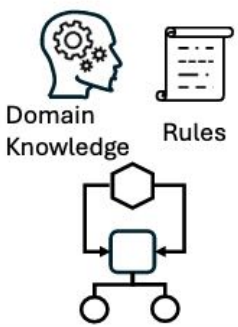
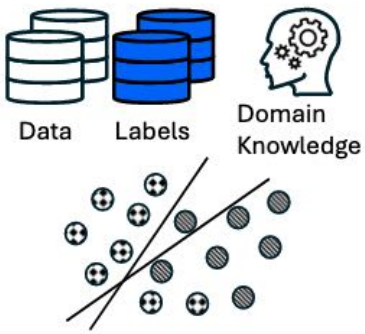
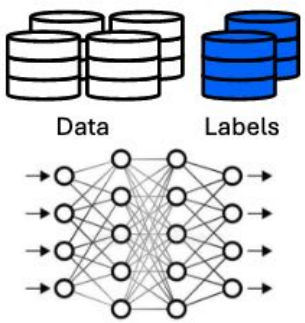
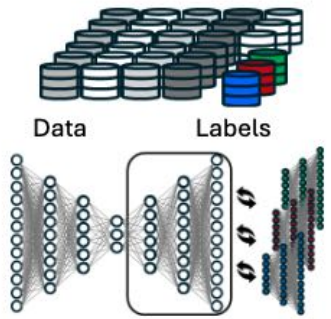
Definition

(Less formal). In particular, we define machine learning as a set of methods that can automatically detect patterns in data and then use the uncovered patterns to predict future data or to perform other types of decision-making under uncertainty.

- Data
- Algorithm/Model
- Evaluation/generalization
- Automation

Machine Learning: Why and What V

Machine and deep learning is a very broad and practical topic. Therefore, this lecture only covers the most basic and ready-to-use ones in the power system. Many of the ideas can be used for more advanced topics.

	Expert Systems	Machine Learning	Deep Learning	Foundation Model
				
Model Size	Very small	Small	Large	Very Large
Features	Hand-designed	Hand-designed	Learnt	Learnt
Learning	None	Supervised	Supervised	Self-supervised
Data	Very few	Few labeled Data	Labeled data	Very large unlabeled + small labeled data
Adaptability	None	Little	Medium	Large

Machine Learning: Why and What VI

Figure: The evolution of AI (Source: [Hamann et al., 2024]). This course mainly focuses on the **machine learning** (with a little time series foundation model) part. The ideas are shared for deep learning and foundation model.

Machine Learning: Why and What VII

A little bit formal definition:

Definition

A computer program is said to learn from experience E with respect to some class of task T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Based on the definition, machine learning algorithms can be classified according to different tasks (T), experience (E), and performances (P),

- Based on the **learning task**, we have
  - *Regression Task*: the computer program is asked to predict a **numerical** value given some input. To solve this task, the learning algorithm is asked to output a function f: $\mathbb{R}^D \rightarrow \mathbb{R}^I$.
  - *Classification Task*: the computer program is asked to specify which of k categories some input belongs to. To solve this task, the learning algorithm is usually asked to produce a function $f : \mathbb{R}^D \rightarrow \{1, \ldots, k\}$. Sometimes, f can produce a **probability distribution** over classes.

Machine Learning: Why and What VIII

- Based on the kind of **experience** the data can have during training, we have
  - Supervised Learning
  - Unsupervised Learning
  - Reinforcement Learning (will not be covered).
- In order to **evaluate** the abilities of a machine learning algorithm, we must design various quantitative measures of its performance.

Machine Learning: Why and What IX

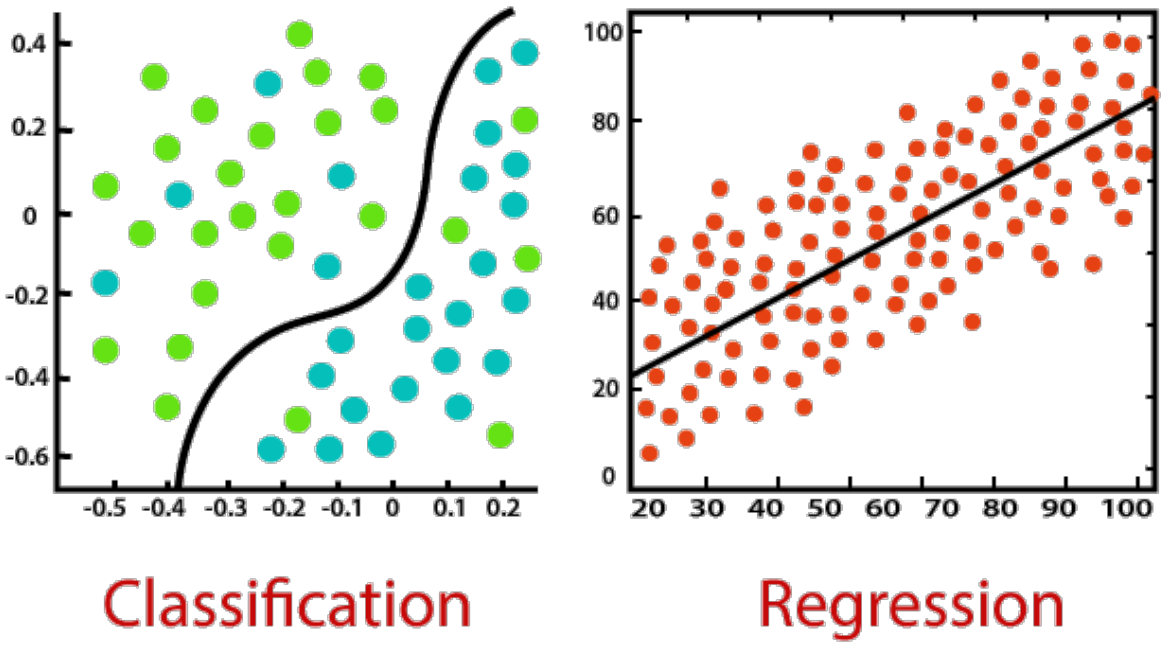


Figure: Regression vs classification. Source: https://www.javatpoint.com/regression-vs-classification-in-machine-learning

Machine Learning: Why and What X

Question

Determine the tasks of the following activities in power system (regression or classification?):

1. Renewable generation forecast.
2. Detect false data injection attack.
3. Predict the optimal dispatch plan of generator.
4. Determine if the current operational point is stable or not.

Question

Determine the experience of the following activities in power system (supervised or unsupervised?):

1. Train renewable generation forecaster based on historical data.
2. Find the common pattern of UK's wind generation in summer.

Outline

Copyright and Reference I

Some of the materials (including images and mathematical definitions) in this lecture note are taken from the following references:

- Murphy, K. P. Machine Learning–A probabilistic Perspective. The MIT Press, 2012.
- Ian Goodfellow, Yoshua Bengio, and Aaron Courville, Deep Learning. The MIT Press, 2016.
- Bishop, Christopher M., and Nasser M. Nasrabadi. Pattern recognition and machine learning. Vol. 4. No. 4. New York: springer, 2006.

You are welcome (but not compulsory) to study online. For example,

- Machine learning specialization by Andrew Ng[1].

[1] https://www.youtube.com/playlist?list=PLkDaE6sCZn6FNC6YRfRQc_FbeQrF8BwGI

Outline

Coursework Overview I

This lecture will take a closer look on the details of machine learning and how to build a successful ML pipeline for power system tasks (e.g. the coursework!).

The coursework **may** include (you will be assigned the coursework later)

- Regression task: predict the output of DC-OPF.
- Classification task: detect on a false data injection attack in power system state estimation.
- Using time series foundation model (TSFM) for wind/solar/price forecasting with real TSO dataset.

Note that the above topic may change, but the ML techniques are the same and will be covered in this lecture.

Coursework Overview II

The coursework will include both conceptual, mathematical questions and programming tasks. Some questions are from the lecture note. The programming tasks will be run as a competition. I.e., each group (two students) should upload their best forecast results, and I will run the grading algorithm for the final score.

You may use any programming language, for example Python or Matlab, for the coursework. However, data will be allocated in Python `.nat` (`numpy`) format only.

You are **not** asked to implement the ML algorithm from beginning. Instead, use well-developed function in Matlab machine learning toolbox or Python sklearn (will be covered later).

Outline

Overview I

Definition

In *supervised learning* approach, the goal is to learn a mapping from inputs x to output y, given a **labeled set of input-output pairs** $\mathcal{D} = \{(x_i, y_i\}_{i=1}^N$. Here $\mathcal{D}$ is the *training set*, and N is the number of training examples.

Each x_i is a D-dimensional vector of numbers, representing, say, the power injection and flow measurements from the RTUs. These are called *features* or *attributes*. They are stored in an $N \times D$ *design matrix* X.

$$X = \begin{pmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{pmatrix} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^D \\ x_2^1 & x_2^2 & \cdots & x_2^D \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^D \end{pmatrix} \in \mathbb{R}^{N \times D}$$

In principal, x_i can contain complex information, such as an image, sentence, etc. In this lecture, we mainly focus on **time series** data.

Overview II

Questions

If you want to build a machine learning model to forecast solar generation, what can be included in X?

Depending on the format of the label y, we have

- y_i is real-valued: *regression* or *pattern recognition* task.
- y_i is categorical: *classification*.

Outline

Linear Regression: Scalar Case I

One of the most widely used models for regression is known as *linear regression*. This asserts that the response is a linear function of the inputs.

$$y(x) = w^T x + \epsilon = \sum_{j=1}^{D} w_j x_j + \epsilon$$

where D is the number of features and ϵ is the residual error between the linear predictions and the true response. y is a **scalar**. w is the model parameter that you want to learn.

We often assume that ϵ has a Gaussian distribution. e.g., $\epsilon \sim \mathcal{N}(\mu, \sigma^2)$. Then the linear regression can be denoted as

$$p(y|x, \theta) = \mathcal{N}(y|\mu(x), \sigma^2(x))$$

Linear Regression: Scalar Case II

In this case, it is assumed that y follows a conditional Gaussian distribution with mean given by

$$\mu(x) = w^T x$$

and the variance equals to the **fixed** noise $\sigma^2(x) = \sigma^2$.

For example, suppose the input is one-dimensional,

$$\mu(x) = w_0 + w_1 x = w^T x$$

where w_0 is the *bias* term, w_1 is the slope, and we can defined the vector $x = (1, x)$.

Questions

Can "linear" regression capture nonlinear relationships?

Linear Regression: Scalar Case III

The linear regression can capture nonlinear relationship between x and y.

$$p(y|x,\theta) = \mathcal{N}(y|w^T\phi(x), \sigma^2)$$

where $\phi(x)$ is a **nonlinear** function of x. For example, a *polynomial regression* is defined as

$$\phi(x) = [1, x, x^2, \cdots, x^d]$$

Linear Regression: Scalar Case IV

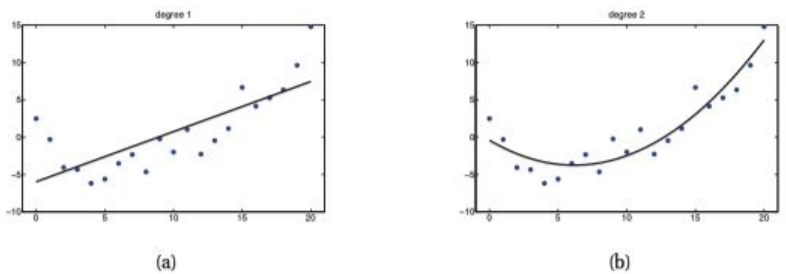


Figure: Linear regression (a) vs nonlinear regression (b).

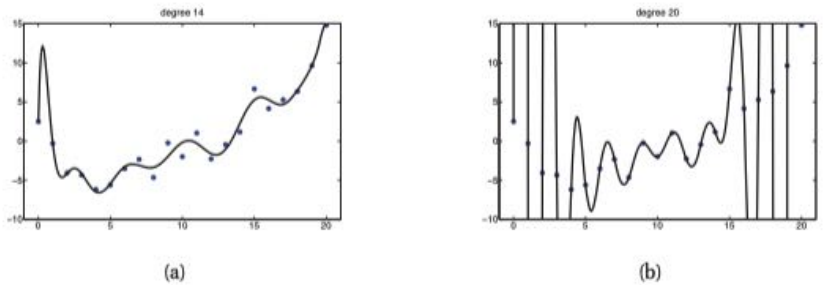


Figure: Polynomial of degrees 14 (a) and 20 (b).

Questions

Does a perfect model always give you good decision?

Linear Regression: Scalar Case V

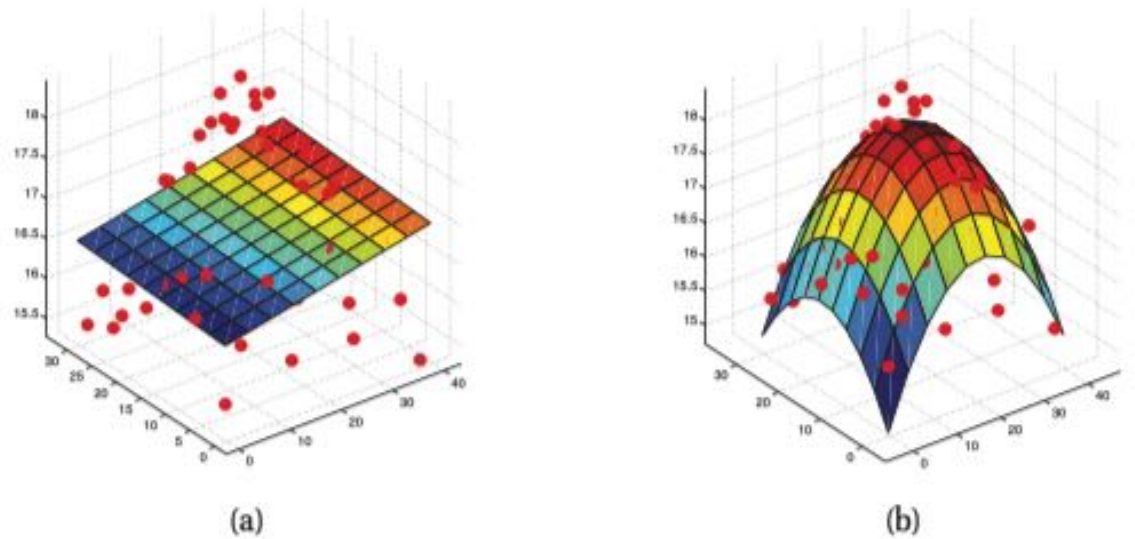


Figure: Linear regression on 2D data. (a). $\mu(x) = w_0 + w_1 x_1 + w_2 x_2$; (b). $\mu(x) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2$

Linear Regression: Maximum Likelihood Estimation I

Linear regression can be modelled and trained by *maximum likelihood estimation* (MLE).

$$\hat{\theta} = \arg\max_{\theta} \log p(\mathcal{D}|\theta)$$

Assuming that the training examples are independent and identically distributed (iid), the log-likehood is represented as

$$\log p(\mathcal{D}|\theta) = \log \prod_{i=1}^{N} p(y_i|x_i, \theta) = \sum_{i=1}^{N} \log p(y_i|x_i, \theta)$$

Recall that a Gaussian distribution is assumed:

$$p(y|x, \theta) = (2\pi\sigma^2)^{-\frac{1}{2}} \cdot e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Linear Regression: Maximum Likelihood Estimation II

Plugging into the log likelihood:

$$\ell(\theta) = -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - w^T x_i)^2 - \frac{N}{2}\log 2\pi\sigma^2$$

In the case when σ is fixed, the second terms is removed. The so-called *mean squared error* (MSE) loss is derived:

$$\min_w \text{MSE}(w) := \sum_{i=1}^{N}(y_i - w^T x_i)^2$$

which is also named as *least squares*.

Question

Can you derive the MSE loss by yourself?

Linear Regression: Maximum Likelihood Estimation III

The MSE loss becomes:

$$\text{MSE}(w) = \frac{1}{2}\|y - Xw\|_2^2 = \frac{1}{2}(y - Xw)^T(y - Xw)$$

where $y \in \mathbb{R}^N$, $X \in \mathbb{R}^{N \times D}$, $w \in \mathbb{R}^D$.

Taking the derivative with respect to w results in the first-order optimality condition:

$$X^T y - X^T X w = 0$$

Therefore, the least-square solution is given as:

$$\hat{w}_{ls} = (X^T X)^{-1} X^T y$$

Questions

Under what condition the $X^T X$ is invertible (non-singular)? What if it is not invertible?

Outline

Logistic Regression I

Logistic "regression" is a **binary classification** (though it is named as regression)...

Let's say $y \in \{0, 1\}$. The output of the logistic regression is the **probability** of one of the class. Therefore, we need

$$\mu(x) = \text{sigm}(w^T x) \in [0, 1]$$

A *sigmoid function* or *logistic function* is defined

$$\text{sigm}(\eta) = \frac{1}{1 + \exp(-\eta)} = \frac{e^\eta}{e^\eta + 1}$$

For the scalar case, let's assume that the output is the probability of class 1,

$$p(y_i = 1 | x_i, w) = \text{sigm}(w_0 + w_1 x)$$

Logistic Regression II

We say a sample is classified as 1 if it has probability larger than 0.5:

$$\hat{y} = 1 \Leftrightarrow p(y = 1|x) > 0.5$$

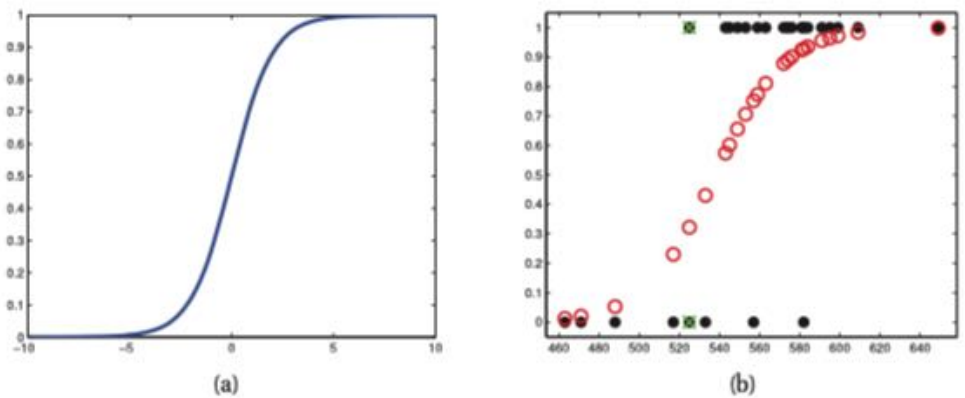


Figure: (a). The sigmoid function; (b). The output of the logistic regression and classification outcomes. The black dots are the input data. The red circles are the predicted probabilities.

Logistic Regression III

The log-likelihood of logistic regression is *cross-entropy* loss:

$$\mathrm{CE}(w) = -\sum_{i=1}^{N} y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i)$$

where $y_i \in \{0, 1\}$. μ_i is the probability of class 1. Therefore, when $y_i = 1$, only the first-term is active (the probability of class 1); and when $y_i = 0$, only the second-term is active (the probability of class 0).

Unlike linear regression (MSE loss), cross-entropy loss does not have a closed-form solution (Why?). Numerical optimization techniques, such as *gradient descent* or *Newton's method* can be used.
The gradient of cross entropy loss is:

$$g = \frac{d}{dw} \mathrm{CE}(w) = \sum_i (\mu_i - y_i) x_i = X^T (\mu - y)$$

Logistic Regression IV

where μ should be understand as element-wise sigmoid function on Xw.

Question

Can you derive the gradient?

Then the *gradient descent* is the following iteration:

$$w_{k+1} = w_k - \eta \cdot g_k$$

where η is a *hyperparameter* that needs to be determined before training (we will come back to this point later).

Question

What happens when η is too large or too small?

Outline

Support Vector Machine I

Support vector machines (SVMs) are **supervised** *max-margin* models with associated learning algorithms that analyze data for **classification** and **regression** analysis.

In addition to linear classification, SVMs can perform **non-linear** classification using the kernel trick (we will not cover this in lecture).

Support Vector Machine II

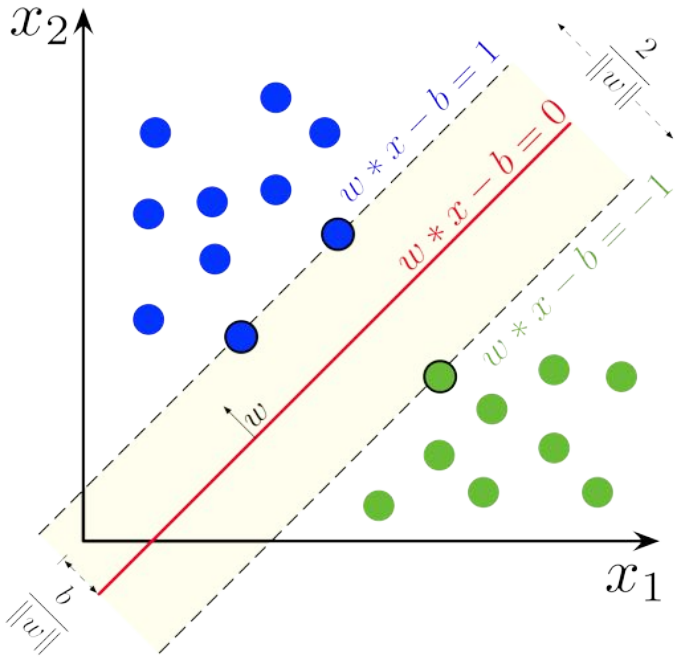


Figure: Max-margin idea in SVM. Source: By Larhmam - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=73710028

Support Vector Machine III

We want to find a hyperplane (the red line in 2D) that divides the two groups of data (blue and green dots). E.g., the distance between the hyperplane and the nearest point (the support vector) from either group is maximized.

Support Vector Machine IV

If the training data is linearly separable (all the data can be eventually perfectly classified!), we can have two parallel hyperplanes that separate the two classes of data with largest distance. The largest distance is the margin.

When we have a normalized dataset (e.g., all data falls in range $[0, 1]$, etc), the two parallel hyperplanes can be written as

$$w^T x - b = 1$$
$$w^T x - b = -1$$

The distance between two hyperplanes is $\frac{2}{\|w\|}$. Therefore, maximizing the margin is equivalent to minimizing $\|w\|$. The distance requires some math to derive, feel free to explore online[2].

Support Vector Machine V

We also need to put data points outside of the margin area, e.g.,

$$w^T x_i - b \geq 1, \quad y_i = 1$$
$$w^T x_i - b \leq -1, \quad y_i = -1$$

which can be compactly written as

$$y_i(w^T x_i - b) \geq 1, \quad \text{for any data}$$

Now we have the objective (to maximize the margin) and constraints (to put data outside the margin area), we can formulate a **optimization problem**:

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}\|w\|^2 \\ \text{s.t.} \quad & y_i(w^T x_i - b) \geq 1, \quad \text{for any data} \end{aligned}$$

Support Vector Machine VI

Questions

Is the SVM formulation a convex optimization problem, why?

As we mentioned earlier, there are some extensions to the hard-margin SVM:

- *Soft-margin SVM* allows some data inside the margin area.
- *Nonlinear or kernel SVM* allows to separate more complex data pattern.

In the coursework, you can test all the different settings (or hyperparameters) using Python packages such as `sklearn`[3], without knowing the detailed math behind them.

[2] `https://www.akshayagrawal.com/lecture-notes/html/hyperplanes.html`
[3] `https://scikit-learn.org/1.5/modules/svm.html`

Outline

Unsupervised Learning: Definition I

Questions

Given a set of power system measurement data, let us consider a task to separate FDI attacked measurements. What can you do if there is **no label** given?

Definition

In *unsupervised learning*, there is only given inputs $\mathcal{D} = \{x_i\}_{i=1}^N$ and the goal is to find interesting patterns in the data. This is a much less well-defined problem, since we are not told what kinds of pattern to look for.

Unsupervised Learning: Definition II

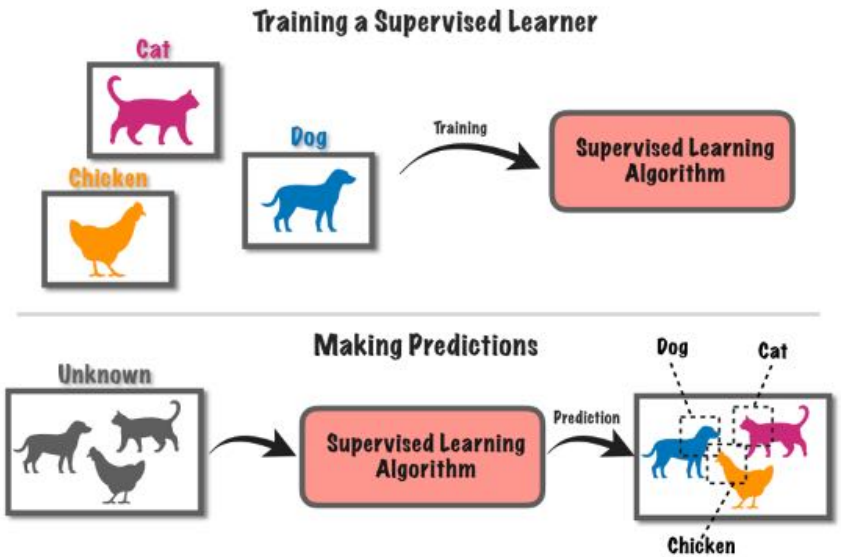


Figure: Supervised vs unsupervised learning. Source: `https://towardsdatascience.com/supervised-vs-unsupervised-learning-in-2-minutes-72dad148f242`.

Some examples include *principal component analysis (PCA)*, *k-means*, etc.

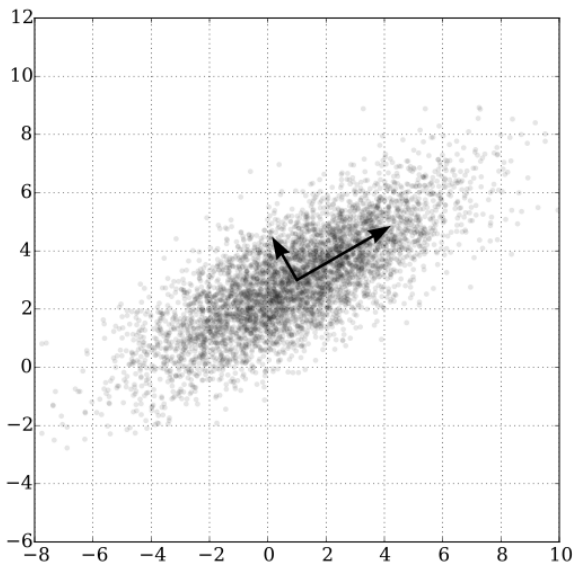
Outline

PCA I

Imagine your have a dataset with 10,000 number of features. And you would like to "compress" the dataset into lower dimensions.

Question

Consider the 2D data shown below. For the two-marked directions, which direction contains more information, why?



PCA II

PCA[4] is a **linear dimensionality reduction** method that can project the data into fewer dimensions (the D) in a way that most of the information of the data is kept!

- Minimize the dimension while keeping the information.

Consider that your power system measurement data has large number of features, e.g., D is very large,

- You would like to visualize the data. Then...
- You would like to first extract useful information, then apply ML algorithms. Then...

Hint: It is always a great practice to visualize your data (in low dimensions); You can also try PCA in coursework!

[4] `https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html`

Outline

k-means Clustering

As the name suggests, the k-means[5] method divides the training set into k different classes in an **unsupervised** way.

The k-means algorithm works as follows

1. Determine the number of clusters k.
2. Initialize k different center of clusters $\{c_1, \cdots, c_k\}$.
3. Assign each training example to cluster i, where i is the index of the nearest center c_i.
4. Each center c_i is updated to the mean of all training examples assigned to cluster i.
5. Repeat step (3)-(4).

Question

For the task of detecting FDI attacks from unlabeled data, how many clusters should be assumed in step (1)?

[5] https://scikit-learn.org/1.5/modules/generated/sklearn.cluster.KMeans.html

Outline

Reinforcement Learning

There is a third type of machine learning, known as *reinforcement learning*, which is somewhat less commonly used. This is useful for learning how to act or behave when given occasional reward or punishment signals. We will not cover this type of ML in this lecture and the coursework.

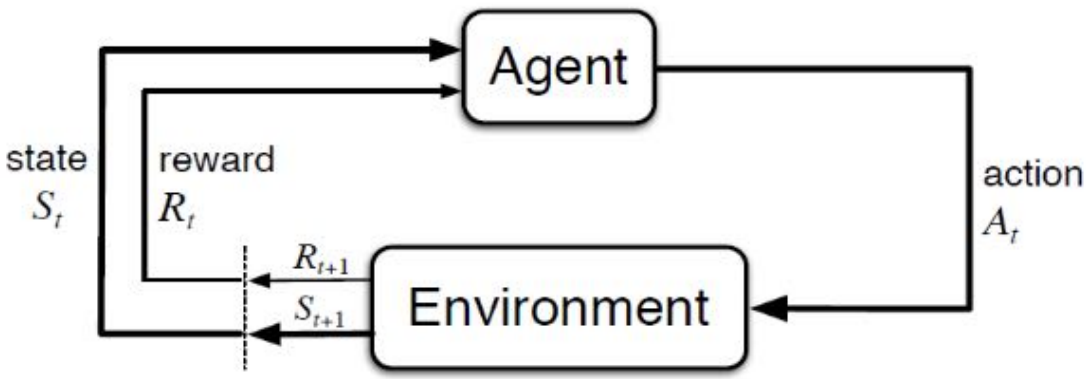


Figure: The reinforcement learning updates the agent by continuously interacting with the environment.

Outline

Performance Measure I

In order to evaluate the abilities of a machine learning algorithm, we must design a quantitative but straightforward measure of its performance.

For *regression task*, we can use the mean squared error (MSE) as defined before.

For the binary classification task on FDI attack, we can define more performance measures, including

- *True positive rate (TPR)*: the proportion of FDI attacks (class 1) that are correctly marked (as class 1). You can also call it the detection rate.
- *False positive rate (FPR)*: the proportion of normal measurement (class 0) that are incorrectly marked (as class 1). You can also call it false alarm.

Performance Measure II

- *True negative rate (TNR)*: the proportion of normal measurements (class 0) that are correctly marked (as class 0).
- *False negative rate (FNR)*: the proportion of FDI attacks (class 1) that are incorrectly marked as (class 0). You can also call it missing alarm rate.

How to remember? FPR: falsely classified as positive, etc.
To systematically include all the measures, the F_1 score is defined as

$$F_1 = \frac{2TP}{2TP + FP + FN}$$

Performance Measure III

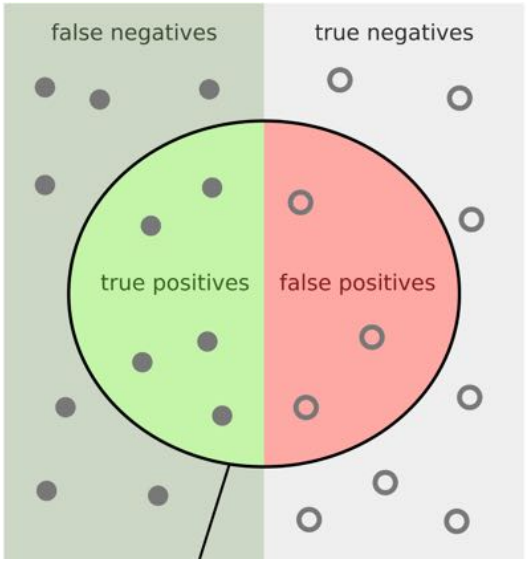


Figure: Performance measure for classifications. The left part represents positive samples (FDI attacks) and the right part represents the negative samples (Normal measurements). The middle cycle represents the detected positive samples.

Question

Can you identify the TPR, FPR, TNR, and FNR in the above plot?

Outline

Overfitting and Underfitting I

Having good accuracy on the training dataset is not the ultimate goal of machine learning. The central challenge in machine learning is that we must perform well on **new, unseen** inputs.

The ability to perform well on previously unobserved inputs (you can call it test set) is called *generalization*.

When training a machine learning model, we **only** have access to a training set, we can compute some error measure on the training set called the *training error*, and we reduce this training error as described in the linear regression case through optimization.

$$\text{MSE}^{\text{train}} = \|X^{\text{train}} w - y^{\text{train}}\|_2^2$$

Overfitting and Underfitting II

What separates machine learning from optimization is that we want the generalization error, also called the *test error*, to be low as well.

$$\text{MSE}^{\text{test}} = \|X^{\text{test}} w - y^{\text{test}}\|_2^2$$

Overfitting and Underfitting III

Therefore, the factors determining how well a machine learning algorithm will perform are its ability to:

1. Make the training error small.
2. Make the gap between training and test error small.

Definition

Underfit occurs when the model is not able to obtain a sufficiently low error value on the training set. *Overfit* occurs when the gap between the training error and test error is too large.

Overfitting and Underfitting IV

We can control whether a model is more likely to overfit or underfit by altering its *capacity*.

- Models with insufficient capacity are unable to solve complex tasks.
- Models with high capacity can solve complex tasks, but when their capacity is higher than needed to solve the present task, they may overfit.

One way to control the capacity of a learning algorithm is by choosing its *hypothesis space* , the set of functions that the learning algorithm is allowed to select as being the solution.

As mentioned before, the linear regression algorithm has the set of all linear functions of its input as its hypothesis space. We can generalize linear regression to include polynomials (polynomial regression), rather than just linear functions, in its hypothesis space. Doing so increases the capacity of the model.

Overfitting and Underfitting V

Normally, we can start to choose model with **lower** capacity (complexity). For example, a linear regression with polynomial of degree one:

$$\hat{y} = b + wx$$

By introducing x^2 as another feature, we increase the complexity of the regression model:

$$\hat{y} = b + w_1 x + w_2 x^2$$

We can continue to add more powers of x, for example a polynomial of degree of 9:

$$\hat{y} = b + \sum_{i=1}^{9} w_i x^i$$

Overfitting and Underfitting VI

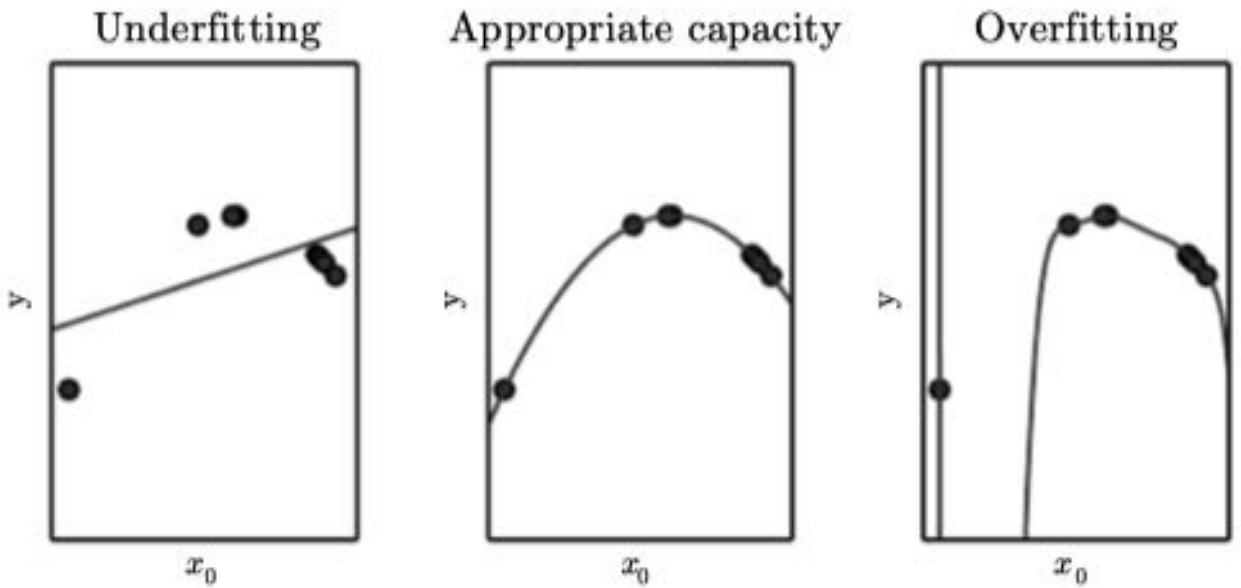


Figure: Underfit vs overfit

Overfitting and Underfitting VII

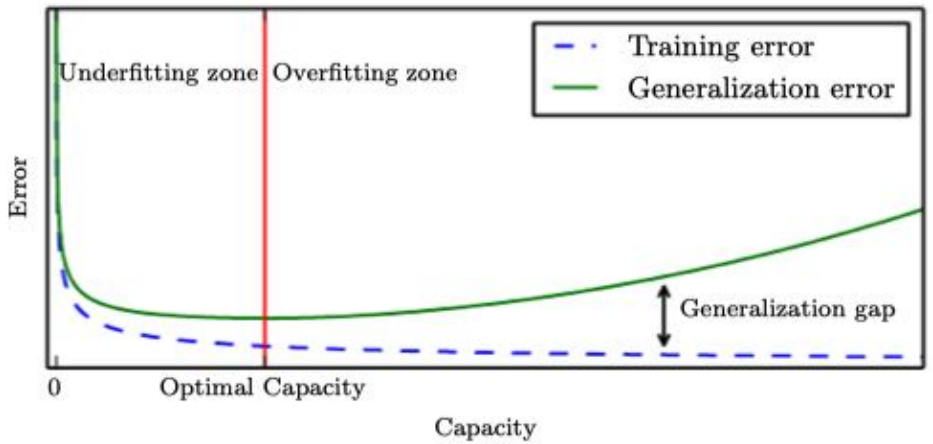


Figure: Typical relationship between capacity and error.

Question

We still have many unsolved problems. For example, we don't have access to the test set... Then how can we know the generalization error (or the performance on test dataset) during training?

Outline

Regularization I

Degree of complexity: So far, the only method of modifying a learning algorithm is to increase or decrease the model's representational capacity by adding or removing the degree of the features.

Larger hypothesis space: Another way to control the performance (capacity) of the algorithms is to choose what kind of functions that can better fit on the data. For example, linear regression would not perform very well if we try to use it to fit on $\sin(x)$ from x.

Regularization: We can introduce a *preference* in the learning algorithm for certain solutions within its hypothesis space. In other words, the algorithm will choose a less preferred (more complex) solution only if it fits the training data significantly better than the preferred (simpler) one.

Regularization II

We can include the *weight decay* on the linear regression loss for *regularization* purpose.

$$\text{MSE}^{\text{reg}} = \text{MSE}^{\text{train}} + \lambda w^T w$$

where λ is a value chosen before the final training (a hyperparameter).

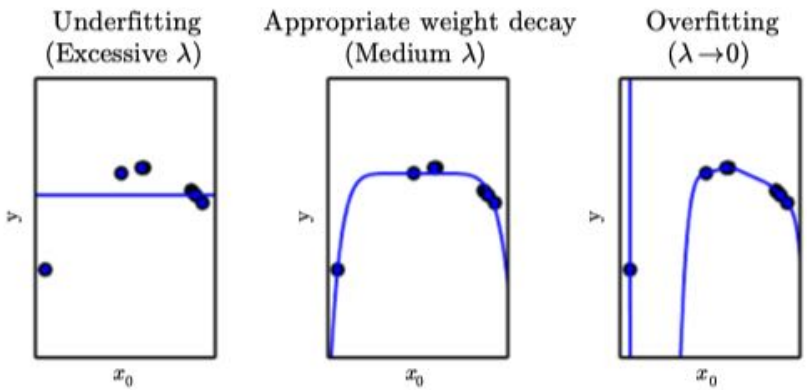


Figure: Different λ on the overfitted polynomial.

Questions

What actually happens if $\lambda \to 0$ and ∞?

Outline

Hyperparameters I

Definition

Most machine learning algorithms have several settings that we can use to control the behavior of the learning algorithm. These settings are called *hyperparameters*.
The values of hyperparameters are **not** adapted by the learning algorithm itself.

The hyperparameters significantly influence the performance of the ML model. For example,

1. In the polynomial regression, $\phi(x) = [1, x, x^2, \cdots, x^d]$, the degree of the polynomial, which represents the **capacity** hyperparameter.
2. In the regression with weight decay, $\mathrm{MSE}^{\mathrm{reg}} = \mathrm{MSE}^{\mathrm{train}} + \lambda w^T w$, the λ value used to control the **strength** of weight decay is another example of hyperparameter.
3. Whenever you train an ML model, there always exists a set of hyperparameters which should carefully play with.

Hyperparameters II

SVC

```
class sklearn.svm.SVC(*, C=1.0, kernel='rbf', degree=3, gamma='scale',
coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200,
class_weight=None, verbose=False, max_iter=-1, decision_function_shape='ovr',
break_ties=False, random_state=None)                                [source]
```

Figure: Sklearn SVM function. There are many hyperparameters to be set. Some of them can be more impactful than the other.

Question

In the simplest setting, it is not appropriate to learn the hyperparameters on the training set. Based on our discussion on overfitting, explain why.

Outline

Validation Set I

Recall a previous problem,

Question

We still have many unsolved problems. For example, we don't have access to the test set... Then how can we know the generalization error (or the performance on test dataset) during training?

We would like to **estimate** the generalizability of the ML model in **an unknown dataset**. The solution is to separate a held-out set from the **training dataset**, called *validation set*. Important notice:

1. The validation set should **NOT** be used to train the model!
2. **NO** test data should be included in the validation set!

Specifically, we split the training data into two disjoint subsets. One of these subsets is used to learn the parameters (e.g., 80%). The other subset is our validation set (e.g., 20%), used to estimate the generalization error during or after training, allowing for the hyperparameters to be updated accordingly.

Validation Set II

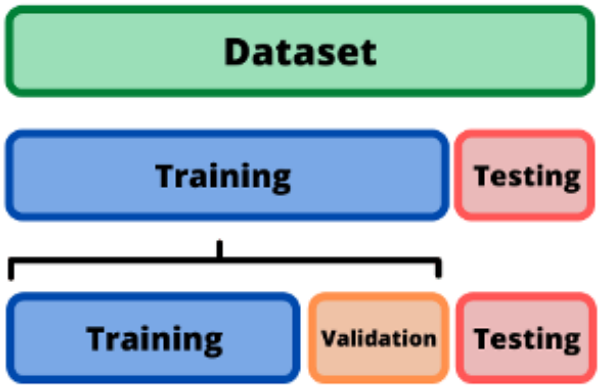


Figure: Train, validation, and test dataset.

For example, in the coursework, you will be asked to train an ML detector to detect FDI attacks. You will be provided with labeled train dataset and unlabeled test dataset.

1. Split the training dataset into 'training dataset' and validation set with a predefined ratio (e.g., 0.8 vs 0.2).
2. Determine an ML model you would like to train on.

Validation Set III

3. Set a list of value of all hyperparameters. E.g., $\lambda = [0, 0.01, 0.001]$, $d = 1, 2, \cdots$ etc.
4. Train the ML model under each of the hyperparameters combination, e.g. $(\lambda = 0, d = 1), (\lambda = 0.01, d = 2)$, etc on the **training dataset**. This processing is also called *grid search*.
5. Evaluate the performance of all trained models with different hyperparameter combinations on **validation set**. The one with the best performance is the final model.

Basically, you never touch on the test set during model training.

Validation Set IV

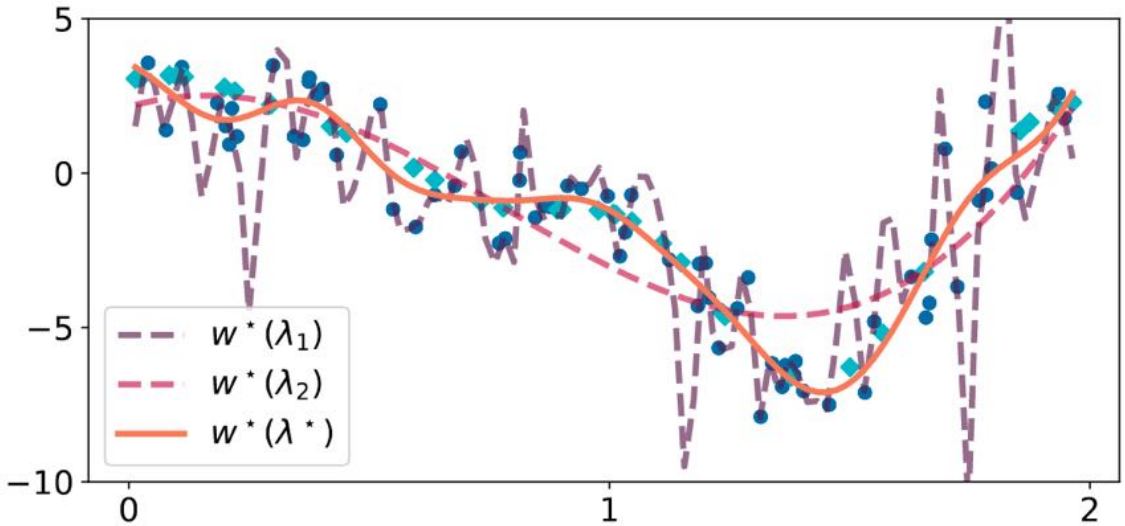


Figure: Tuning hyperparameter λ based on the performance on the **validation set**. This example is taken from [Blondel and Roulet, 2024]. Blue dots are training samples and clan dots are validation samples.

Question

Can you tell which fitting curve is over-fitted and under-fitted?

Outline

No Free Lunch Theorem I

- "All models are wrong, but some models are useful."
- There is no single best model that works optimally for all kinds of problems. The reason is that a set of assumptions that works well in one domain may work poorly in another.
- As a consequence of the no free lunch theorem, we need to develop many different types of models, to cover the wide variety of data that occurs in the real world. And for each model, there may be many different algorithms we can use to train the model.
- But with the development of foundation model, the No Free Lunch Theorem "seems" to be less accurate.

Outline

Foundation Model I

All the techniques we discussed earlier require training by yourself. This is because one model is typically only good at one task.

Definition

A **foundation model** is a **large-scale**, **pre-trained** model (usually based on deep learning) that learns general-purpose representations from **massive, diverse datasets** and can be **adapted** (fine-tuned or prompted) to perform many downstream tasks.

- Trained on broad and heterogeneous data (e.g., text, image, code. multimodal data, etc);
- Use self-supervised or unsupervised learning (e.g. predicting masked tokens, next word, next frame, etc.): predict on itself.
- Transferable to many domains with prompting (zero-shot) or fine-tuning (few-shot).

Foundation Model II

- **LARGE**: Billions of parameters.

Questions

Can GPT-5 be seen as a foundation model?

Suppose you have a model like GPT-5 trained on global text data. You can immediantely adapt it for:

- Writing power system reports (text generation).
- Extracting entities from energy market documents (information extraction).
- Explaining optimization models (reasoning).

You don't train it from scratch — you just prompt or fine-tune it $\rightarrow$ this reusability makes it a foundation model.

Outline

Time Series Foundation Model (TSFM) I

Definition

A time series foundation model is a large pre-trained model designed to understand and predict **temporal** patterns across diverse time-dependent datasets. It is trained on massive collections of time series from many domains (e.g., finance, energy, weather, health) and can generalize to new, unseen time series without retraining from scratch.

Questions

Does TSFM follow the properties of general FM?

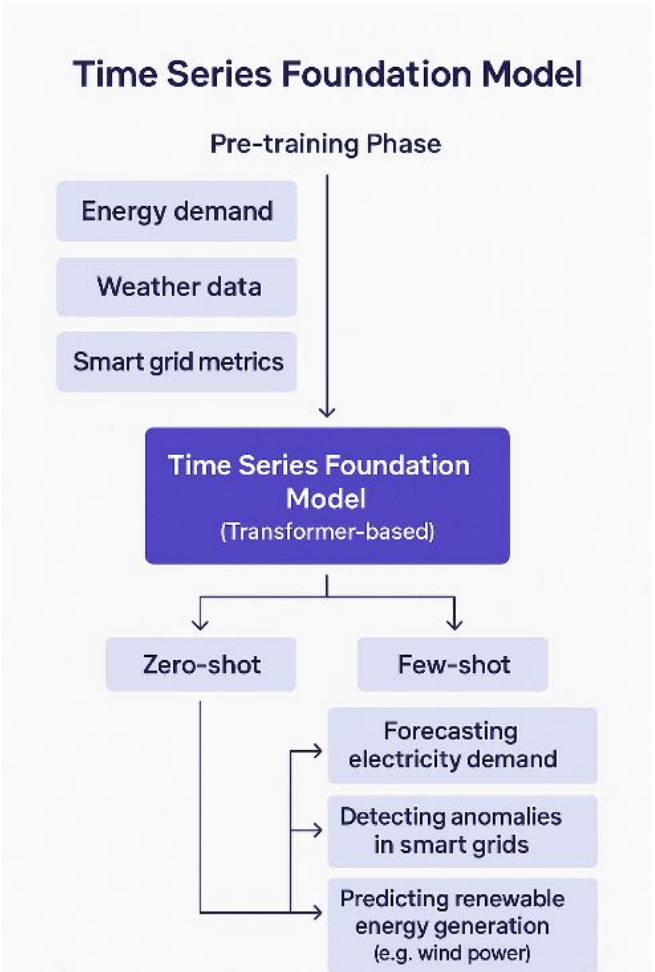
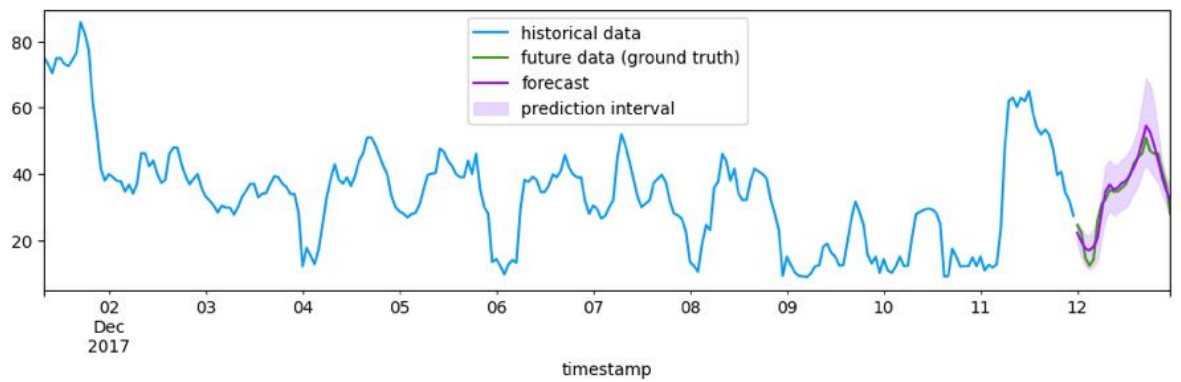


Figure: The concept of TSFM (image generated by GPT-5).

Outline

Amazon Chronos I

- Chronos is a family of pretrained time series forecasting models open sourced by Amazon. The latest version supports zero-shot univariate, multivariate, and covariate-informed forecasting tasks (Can you guess what is covariate?). The largest one has 710M parameters.
- GitHub: `https://github.com/amazon-science/chronos-forecasting`.
- A zero-shot example for energy price forecasting (Open Google Colab).



Outline

Special Topic Two: DATA? DATA!

Where and How to obtain the Data

Why Data is Important? I

- All the previous discussions assume that you already have **sufficient** dataset with **good quality**.
- For power systems, some of the most important data include power consumption and generation, energy price (day-ahead and real-time) in an open market, and operational status such as congestion level.
- Believe it or not, high quality data is not easy to get. And there is a famous one "Garbage in, garbage out" (GIGO).
- But luckily, the EU (including UK) has enforced many regulations for opening data.

European's Effort on Data Transparency I

- Open energy data is essential for ensuring transparency, market efficiency, and innovation in the energy sector.
- It allows regulators, researchers, and consumers to better understand how electricity is produced, transmitted, and consumed, fostering trust and enabling smarter system planning and policy design.
- The European Union has established several key regulations to enforce this transparency, most notably Regulation (EU) No 543/2013, which mandates that electricity market participants, such as transmission system operators (TSOs), power plant operators, and large consumers, publish detailed operational data on generation, demand, outages, and balancing.

European's Effort on Data Transparency II

- Complementary frameworks like REMIT (Regulation 1227/2011) ensure integrity in wholesale energy markets, while newer laws such as the Energy Efficiency Directive (2023/1791) and the EU Data Act (2023/2854) extend transparency and data-sharing obligations to other parts of the energy ecosystem.
- Most of this data is publicly available and freely accessible through the **ENTSO-E Transparency Platform**, which serves as the central hub for Europe-wide electricity system operational data.

Where to Find the Power System Data I

- Electricity generation, transportation and consumption for the European market: `https://newtransparency.entsoe.eu/` is the main source for obtain market, load, generation, transmission, and balancing data.
- Weather dataset is important to forecast nearly all factors in electricity market. You may find it useful in ERA5 dataset `https://cds.climate.copernicus.eu/datasets`.
- More detailed operation and market data may be found on regional operators website, such as FinGrid and Elia.

Reference I


Blondel, M. and Roulet, V. (2024).
The elements of differentiable programming.
arXiv preprint arXiv:2403.14606.


Hamann, H. F., Brunschwiler, T., Gjorgiev, B., Martins, L. S., Puech, A., Varbella, A., Weiss, J., Bernabe-Moreno, J., Massé, A. B., Choi, S., et al. (2024).
A perspective on foundation models for the electric power grid.
arXiv preprint arXiv:2407.09434.