Lecture 5: Logistic Regression
Physics meets ML to solve cosmological inference

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Abstract: The goal of cosmological inference is to learn about the origin, composition, evolution, and fate of the cosmos from all accessible sources of astronomical data, such as the cosmic microwave background, galaxy surveys, or electromagnetic and gravitational wave transients. Traditionally, the field has progressed by designing and modeling intuitive summaries of the data, such as n-point correlations. This traditional approach has a number of risks and limitations: how do we know if we computed the most informative statistics? Did we forget any summaries that would have provided additional information or break parameter degeneracies? Did we take into account all the ways the model is affecting the data? To be feasible, the traditional approach imposes approximations on the statistical modeling (e.g. the likelihood form) and on the physical modeling. I will discuss a new mode of cosmological inference: simulation-based, full-physics modeling, made feasible through multiple advances in 1) machine-learning, 2) in the way we design and run simulations of cosmological observables, and 3) in how we compare models to data. The goal is to use current and next generation data to reconstruct the cosmological initial conditions and constrain cosmological physics much more completely than has been feasible in the past. I will discuss current status, and ways to meet the new challenges inherent in this approach, including robustness to model misspecification.
Recap of Lecture 4

- Linear regression
- Regularization (Ridge, LASSO)
- MLE
- MAP
- Relation of MLE and MAP with Least/Square and Ridge regression
- Linear regression will be replaced by more complicated/non-linear models
- Regression on the 1D Ising model
Outline for today

• Logistic classification (binary classification)
• Binary cross-entropy
• Multi-class classification
• MNIST

References: 1803.08823
Logistic Regression
Logistic Regression

- Discrete variables and not continuous output, determine categories (cat or dog, ordered or disordered phase, SUSY or background).
- Start with binary classification, will generalize later to multi-class.
- Data labels for M classes:
  \[ m \in \{0, \ldots, M - 1\} \]
- Task: predict correct labels/features from input design matrix:
  \[ X \in \mathbb{R}^{n \times p} \quad \text{n samples, p features} \]
- Backbone of modern **supervised deep learning** models.
Linear Classifier

- Categorize data using a weighted linear-combination of features and an additive constant:

\[ s_i = \mathbf{x}_i^T \mathbf{w} + b_0 \equiv \mathbf{x}_i^T \mathbf{w}, \]

**short-hand** \[ \mathbf{x}_i = (1, \mathbf{x}_i) \text{ and } \mathbf{w} = (b_0, \mathbf{w}). \]

- Map output of a linear regression to

\[ \sigma(s_i) = 1 \text{ if } s_i \geq 0 \text{ and } 0 \text{ otherwise} \]

known as perceptron in the ML literature

- Perceptron is not differentiable (hard to train via gradient descent).
The sigmoid function is differentiable, and satisfies some useful properties:

\[
1 - \sigma(s) = \sigma(-s)
\]

\[
\sigma'(s) = \sigma(s)(1 - \sigma(s))
\]

\[
\sigma'(s) = \sigma'(-s)
\]
• Probability that a data point belongs to a category $y_i = \{0, 1\}$:

$$P(y_i = 1|x_i, \theta) = \frac{1}{1 + e^{-x_i^T\theta}}.$$  

$$P(y_i = 0|x_i, \theta) = 1 - P(y_i = 1|x_i, \theta),$$

• Motivated by the two-state system in statistical mechanics:

$$P(y_i = 0) = \frac{e^{-\beta \epsilon_0}}{e^{-\beta \epsilon_0} + e^{-\beta \epsilon_1}} = \frac{1}{1 + e^{-\beta \Delta \epsilon}},$$

$P(y_i = 1) = 1 - P(y_i = 0).$

• In terms of the sigmoid function:

$$P(y_i = 1) = \sigma(x_i^T w) = 1 - P(y_i = 0).$$
Constructing the Loss Function

- The likelihood of observing the data:

\[
P(D|\mathbf{w}) = \prod_{i=1}^{n} [\sigma(\mathbf{x}_i^T \mathbf{w})]^{y_i} [1 - \sigma(\mathbf{x}_i^T \mathbf{w})]^{1-y_i}
\]

- The log-likelihood:

\[
l(\mathbf{w}) = \sum_{i=1}^{n} y_i \log \sigma(\mathbf{x}_i^T \mathbf{w}) + (1 - y_i) \log [1 - \sigma(\mathbf{x}_i^T \mathbf{w})].
\]

- Maximum Likelihood Estimation (MLE):

\[
\hat{\mathbf{w}} = \arg \max_{\theta} \sum_{i=1}^{n} y_i \log \sigma(\mathbf{x}_i^T \mathbf{w}) + (1 - y_i) \log [1 - \sigma(\mathbf{x}_i^T \mathbf{w})].
\]

- The cost (error) function:

\[
C(\mathbf{w}) = -l(\mathbf{w}) = \sum_{i=1}^{n} -y_i \log \sigma(\mathbf{x}_i^T \mathbf{w}) - (1 - y_i) \log [1 - \sigma(\mathbf{x}_i^T \mathbf{w})].
\]

\textit{cross entropy}
**Optimizing the Loss Function**

- The cross entropy is a **convex function** of the weights; any local minimizer is a global minimizer.

- The cross entropy is differentiable, can be minimized via SD:

  \[ 0 = \nabla C(w) = \sum_{i=1}^{n} [\sigma(x_i^T w) - y_i] x_i, \]

- We can supplement the cross entropy with additional **regularizers** such as L^1 and L^2 regularization.

- Modifications such as adding stochasticity (e.g., mini-batches) and momentum discussed in Lecture 3 also apply.
Phases of 2D Ising Model
Phases of the 2D Ising Model

- The Hamiltonian for the 2D Ising Model:
  \[ H = -J \sum_{\langle ij \rangle} S_i S_j, \quad S_j \in \{\pm 1\}, \]

- 2D lattice of L x L spins.

- Periodic boundary conditions.

- Onsager’s exact solution: a phase transition in the thermodynamic limit at the critical temperature:
  \[ T_c/J = 2/\log(1 + \sqrt{2}) \approx 2.26 \]
Phases of the 2D Ising Model

- Can we train a binary classifier to distinguish between two phases of the 2D Ising model?

- We need a dataset, i.e. samples at a given temperature. How do we do this? One common way: Monte Carlo Simulations.

- Our binary classifier misses features like contiguous ordered 2D domains; such info can be incorporated using deep convoluted neural networks (CNNs) and topological data analysis.
Phases of the 2D Ising Model

• Generate a dataset for 40x40 grid using MC simulations to prepare $10^4$ states at every temperature $T$.

• We know which temperatures the samples are from, and their labels (e.g., 0=disordered, 1=ordered).

• What we are doing is called **supervised learning**.

• Later in the course we will see methods which do not need these labels, i.e. **unsupervised learning**.

• For physics in practice: supervised learning can teach you how well a method is working for a desired task. To do something “new”, we usually have to use unsupervised learning.
physicists to help discriminate between the two classes. These high-level features can be thought of as rapidity variables (''features'').

The first 8 features are direct measurements of final state particles, in this case the to contain events with two leptons (electrons or muons).

\[ J \]

we will use the output of our logistic regression to define a part of phase space that is enriched in signal events (see event is from a signal or a background event. Rather than using the kinematic quantities of final state particles directly, to the beam line (the final state particles, for example having one or more leptons with large amounts of momentum that are transverse percentage of signal events. Typically this is done by using a series of simple requirements on the kinematic quantities of processes. Unfortunately, we do not know for sure what underlying physical process occurred (the only information we have access to are the final state particles). However, we can attempt to define parts of phase space that will have a high percentage of signal events. Typically this is done by using a series of simple requirements on the kinematic quantities of the interested reader to play with the different regularization types and numerical solvers in the MLnotebooks.html.

emphasize the role of the regularizers in this section, but they are crucial in order to prevent overfitting. We encourage data (red line).

Indeed, the critical states.) Looking at the states in the near-critical region, c.f. We might expect that the difficulty of the phase recognition problem depends on the temperature of the queried sample. Looking at the states in the near-critical region, c.f. We might expect that the difficulty of the phase recognition problem depends on the temperature of the queried sample.

Fig. 21. 34

According to theory, for the SGD regularization strength \( \lambda \) suggested by the training (blue) and test (red) accuracy curves being very close to each other. Interestingly, the data, we can study the degree of overfitting. The first thing to notice in of the classifier as the percentage of correctly classified data points. Comparing the accuracy on the training and test data, but not on the near-critical data for certain values of the.

We might expect that the difficulty of the phase recognition problem depends on the temperature of the queried sample.

The dataset we are using comes from the UC Irvine ML repository and has been produced using Monte Carlo simulations. It is well-known that near the critical temperature, the ferromagnetic correlation length diverges, which leads for the SGD regularization strength \( \lambda \). Moreover, similar to the linear regression examples, we find that there exists a sweet spot that results in optimal performance of the logistic regressor, at about \( \lambda \). We use both ordered and disordered states to train the logistic regressor for details) to optimize the logistic regression cost function with the critical region. With this in mind, consider the following three types of states: ordered (green) and critical (green) data. The solid and dashed lines compare the 'liblinear' and 'SGD' solvers, respectively.

Experiment with Jupyter Notebook 6:
https://physics.bu.edu/%7Epankajm/MLnotebooks.html
SUSY vs SM Background
SUSY vs SM Background

- Using the dataset from the UC Irvine ML repository produced by MC simulations to contain events with 2 leptons (electrons or muons).

- These events with 2 leptons with large $p_T$ can occur in SUSY models or within the SM.

- 18 kinematic variables (“features”) are recorded for each event.

- Can train a logistic regressor to classify the events into SUSY or SM background.

Figure 4 | Diagrams for SUSY benchmark. Example diagrams describing the signal process involving hypothetical supersymmetric particles $\chi^\pm$ and $\chi^0$ along with charged leptons $\ell^\pm$ and neutrinos $\nu$ (a) and the background process involving $W$ bosons (b). In both cases, the resulting observed particles are two charged leptons, as neutrinos and $\chi^0$ escape undetected.

Baldi et al, Nature Communications, Volume 5, Article number: 4308 (2014)
Fig. 23. ROC curves for a variety of regularization parameters with L2 regularization using TensorFlow (top) or Sci-Kit Learn (bottom).

Fig. 24. Comparison of leading vs. sub-leading lepton $p_T$ for signal (blue) and background events (red). Recall that these variables have been scaled to have a mean of one.

For an alternative mathematical description of the categories, which labels the classes by integers, see [Softmax_Regression](http://ufldl.stanford.edu/wiki/index.php/Softmax_Regression).
Multi-class Classification
Softmax Regression

- Going from 2 labels to M labels.
- Treat the label as a vector \( y_i \in \mathbb{Z}_2^M \), i.e., one hot-encoding of labels:

\[
0 \rightarrow \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad 1 \rightarrow \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \ldots, \quad M - 1 \rightarrow \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}
\]

- The probability of being in class \( m \) is the softmax function:

\[
P(y_{im'} = 1 \mid x_i, \{w_k\}_{k=0}^{M-1}) = \frac{e^{-x_i^T w_{m'}}}{\sum_{m=0}^{M-1} e^{-x_i^T w_m}}
\]

where \( y_{im'} \equiv \{y_i\}_{m'} \) is the \( m' \)-th component of vector \( y \).
Softmax Regression

- Likelihood of this M-class classifier:

\[
P(\mathcal{D}|\{\mathbf{w}_k\}_{k=0}^{M-1}) = \prod_{i=1}^{n} \prod_{m=0}^{M-1} [P(y_{im} = 1|x_i, \mathbf{w}_m)]^{y_{im}} \]
\[
\times [1 - P(y_{im} = 1|x_i, \mathbf{w}_m)]^{1 - y_{im}}
\]

- Cost function:

\[
C(\mathbf{w}) = - \sum_{i=1}^{n} \sum_{m=0}^{M-1} y_{im} \log P(y_{im} = 1|x_i, \mathbf{w}_m) \]
\[
+ (1 - y_{im}) \log (1 - P(y_{im} = 1|x_i, \mathbf{w}_m)).
\]

- Activations (one-hot encoding), can be thought of as activating particular cells (e.g. in your brain).

- Becomes a lot harder for a larger number of classes.
Classifying Digits — MNIST
MNIST

- Classifying digits ⇒ M=10 categories

- MNIST = Dataset of handwritten digits, 28x28=784 pixel grid, each assumes 256 grayscale values, interpolating between white and black.

  Yann LeCun, Corinna Cortes, Christopher Burges

  http://yann.lecun.com/exdb/mnist/

- 60,000 images: 50,000 for training, 10,000 for testing

Experiment with Notebook 7 using softmax:
https://physics.bu.edu/%7Epankajm/MLnotebooks.html
Summary

- Binary classification Logistic sigmoid
- Binary cross-entropy as loss function
- Multi-class classification
- 3 Examples: Phase classification 2D Ising, SUSY datasets, handwritten digits MNIST.