Regression

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Background Picture: NVIDIA GauGAN output by Paragism

Objective | o

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- High level overview of regression and related ML concepts. *Slides*
- Transforming these perspectives into code. *ipynb Demo*

For some, this will be a review; for some, this might be entirely novel content. Those who have questions about the slides are encouraged to address these to their teammates.

History 1

- Statistical 'Regression' was discovered in the early 19th century
- Often discovery has been ascribed to Gauss, Legendre and Sir Francis Galton
- Sir Francis Galton coined the term 'Regression'
- *Regression towards the mean*: The observation that the descendants of tall ancestors, often were shorter than their parents.
 - Interesting: Galton worked on multiple eugenics projects.



Objective

- **Context:** We have numerical data:
 - (\vec{x}_i, y_i) where $x \in \mathbb{R}^d, y \in \mathbb{R} \forall i \in \{1, ..., n\}$
 - In other words, we have features, independent variables decoded as x. The predictor is encoded as a y. Each datapoint is such pair.
 - Example:
 - *x*: square footage, neighborhood, distance to nearest station, number of bedrooms/bathrooms, etc.
 - *y*: rent
- Goal: <u>Predict</u> a <u>numerical outcome</u> *y* by reconstructing the underlying true function.
- **Assumption:** There exists some function that models the true relationship between *x* and *y*.



More Concrete Goal:

We want to find the \hat{a} as close as possible to a in the true function:

$$y = a_1 x_1 + \dots + a_d x_d$$

Linear Regression

- Data 8 perspective (2D):
 - The correlation coefficient ρ turns out to be the slope of the regression line of the variables in standard units.
 - Convert this correlation coefficient ρ to an alpha through multiplying by the ratio of the SD of y and x.
 - Calculate the intercept by plugging in the mean of y and x.
- Minimizing Loss Function Perspective:
 - We can also just try to minimize our loss function, MSE, least squares.
 - Through *Stochastic Gradient Descent*, we can attain the particular weights that minimize the error.



- Linear Algebra Perspective:
 - It turns out that the least square solution by (b):



$$\hat{a} = \frac{argmax}{a} \|Xa - y\|^2$$

This function that minimizes the distance of each residual to the function can also be interpreted as a projection of each point onto a smaller hyperplane.

- MLE Perspective:
 - It also turns out that the *OLS solution* we find, is the most likely to occur given the data that we observe.

$$\hat{a} = \frac{argmax}{a}P(y | X, a)$$

• If you want to know more about the Statistics perspective, ask Ewen!



 However, what happens when we wanted to predict a nonlinear function?



- We can combine turn our feature x into features $x,\,x^2$, called lifting.
- The Kernel trick bypasses the direct need to create this featurization but does put a prior belief on our features, which has consequences.

Regularization 6

- Loss Function: $MSE = \frac{1}{n} \sum_{i=1}^{n} (pred actual)^2 = \frac{1}{n} ||X\widehat{w} y||^2$
 - Can be decomposed into bias² and variance
 - Bias: How well does my model fit the data without noise.
 - Variance: How much noise am I taking into account.



• To counteract *high variance/too much noise*, we **regularize;** add an extra penalty term to the loss function so that weights don't explode:

RIDGE (Complex Models): $\lambda ||w||_2^2$ **LASSO (Parsimony):** $\lambda ||w||_1$

Deep Learning 7

- Nonlinearities are a bottleneck!
- Artificial Neural Networks provide solution:
 - Universal Approximation Theorem states that *neural networks* can approximate any continuous function.
 - Moreover, any neural network with one hidden layer can approximate any real function up to your chosen precision.
- Caveats: High dimensionality \rightarrow Overfitting



Bias, Variance, and?

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- Recall:
 - Traditionally, the MSE can be decomposed as:
 - **Bias**²: How well would my model fit without any noise?
 - Variance: How much contamination do I take into my model?
 - What happens if we have more way more variables in our model than there are in real life for a certain pattern? In other words, what happen if we overparameterize?

Bias, Variance, and Regularization

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 - Summer `19:
 Reconciling modern machine-learning practice and the classical bias-variance trade-off
 Mikhail Belkin, Daniel Hsu, Siyuan Ma, and Sournik Mandal
 PNAS August 6, 2019 116 (32) 15849-15854; first published July 24, 2019; https://doi.org/10.1073/pnas.1903070116
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