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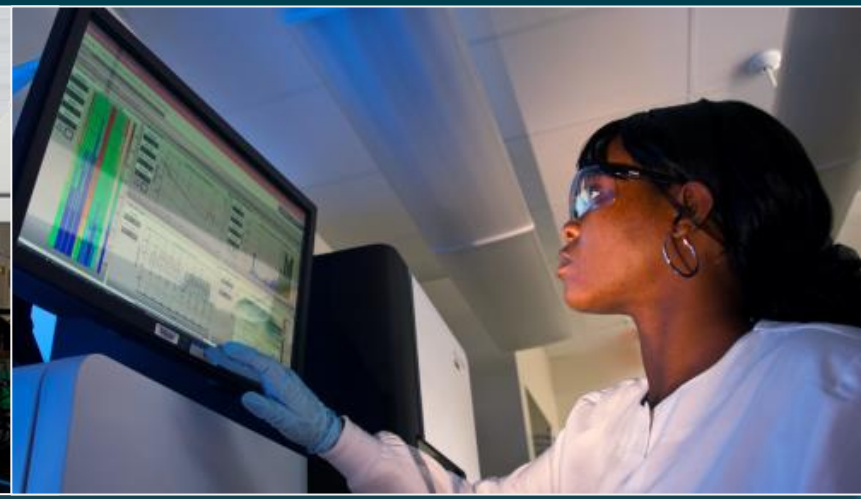

Machine Learning Jargon
An Introduction to Key Concepts and Terms

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Notes

- **<u>Scope:</u> Basic, commonly used machine learning terminology**
- **These terms will be highlighted in yellow**
- **I will focus on what people typically mean or refer to**
- **These are my own opinions**
- **There are nuances to everything**
- **Feel free to ask questions during the presentation:**
  - During the presentation, use the QA feature of Webex
  - We will allow attendees to unmute themselves for questions after the talk is complete
- **Links to slides and recording will be available at the NCI Data Science Learning Exchange (https://cbiit.github.io/p2p-datasci)**
- **Please fill out brief survey on Webex at the end of the talk**

Introduction

- **Machine learning: The science (and art) of programming computers so they can learn from data (Géron)**
  - Minimal explicit programming
- **Examples:**
  - Image processing: Optical character and facial recognition
  - Natural language processing (NLP): Spam filters
  - Bioinformatics: Tumor classification from gene expression data
- **Main types of machine learning:**
  - Supervised learning
  - Unsupervised learning
  - Semi-supervised learning
  - Reinforcement learning

Simple example of supervised learning: linear regression

- **<u>Experiment:</u> 10 random times throughout the day, look out the window, and count all the birds and foxes you see:**

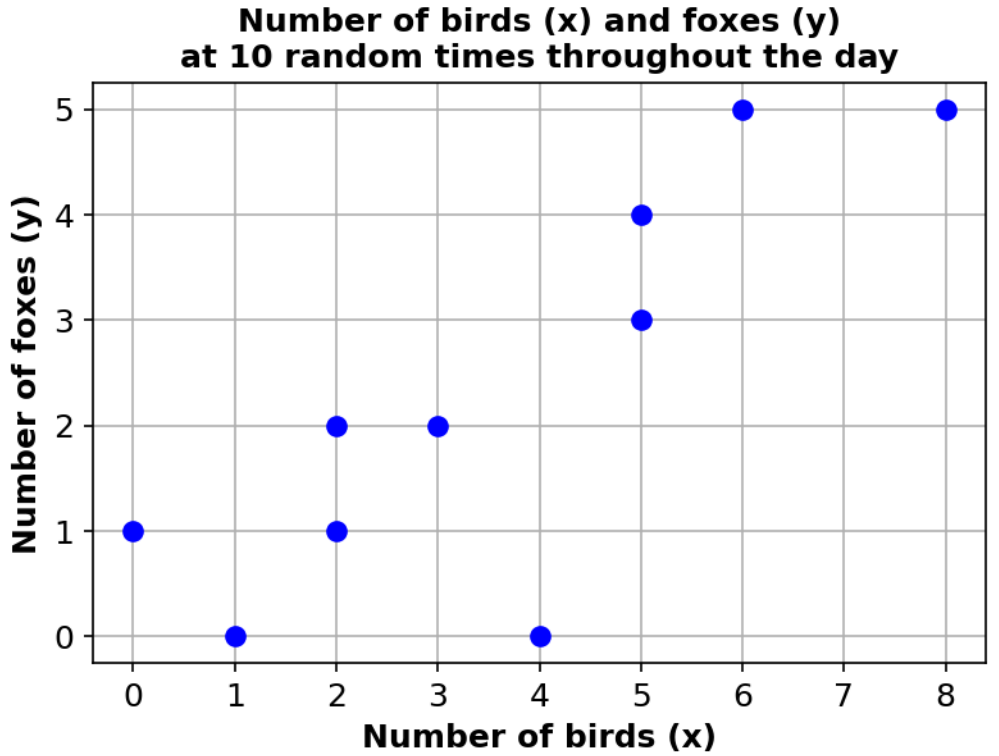
Each observation is called a sample or instance

The dependent variable *y* is called the label or target value

The independent variable *x* is called the feature

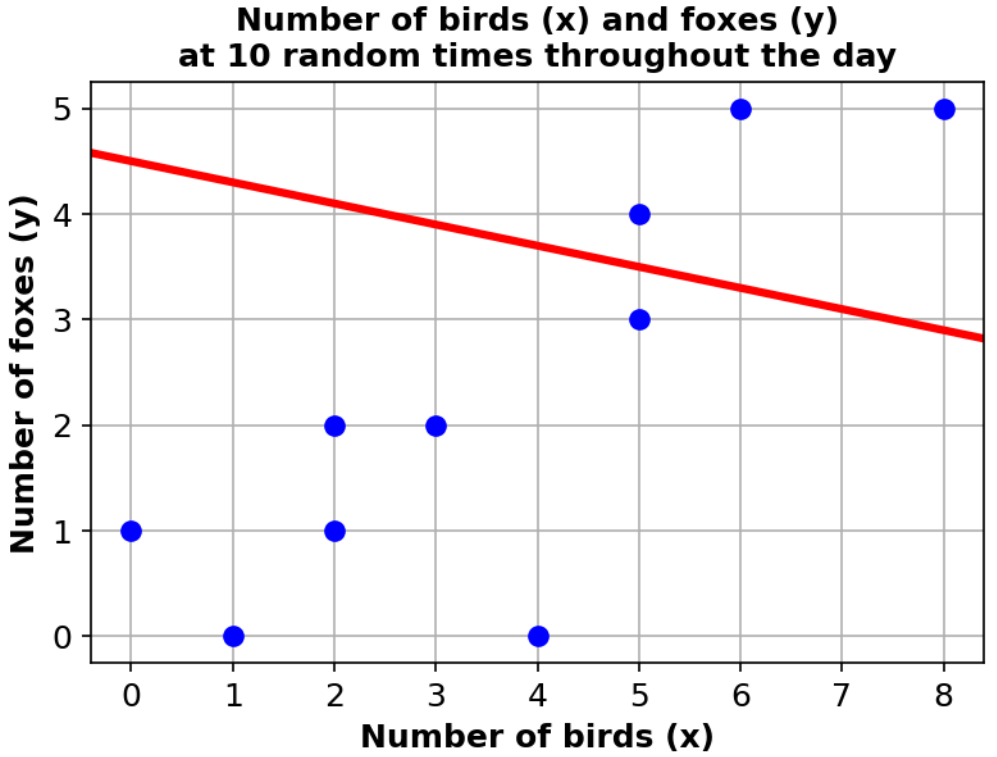
The entire dataset is called the training dataset

Number of birds (*x*)	Number of foxes (*y*)
5	3
2	2
1	0
3	2
6	5
0	1
4	0
2	1
8	5
5	4



Simple example of supervised learning: linear regression, ctd.

- **Question:** Can the number of birds (*x*) be used to predict the number of foxes (*y*)?
- **Approach:** Choose a **model** that relates *x* to *y*
- **Model selection:** The process of specifying the model architecture
- Here, let's select a **linear regression** model:
  $y_{predict}(m, b) = mx + b$
- m and b are called the **weights** or **parameters** of the model
- The process of determining the model's weights that best describe the data (*x* and *y*) is called **training** or **fitting**

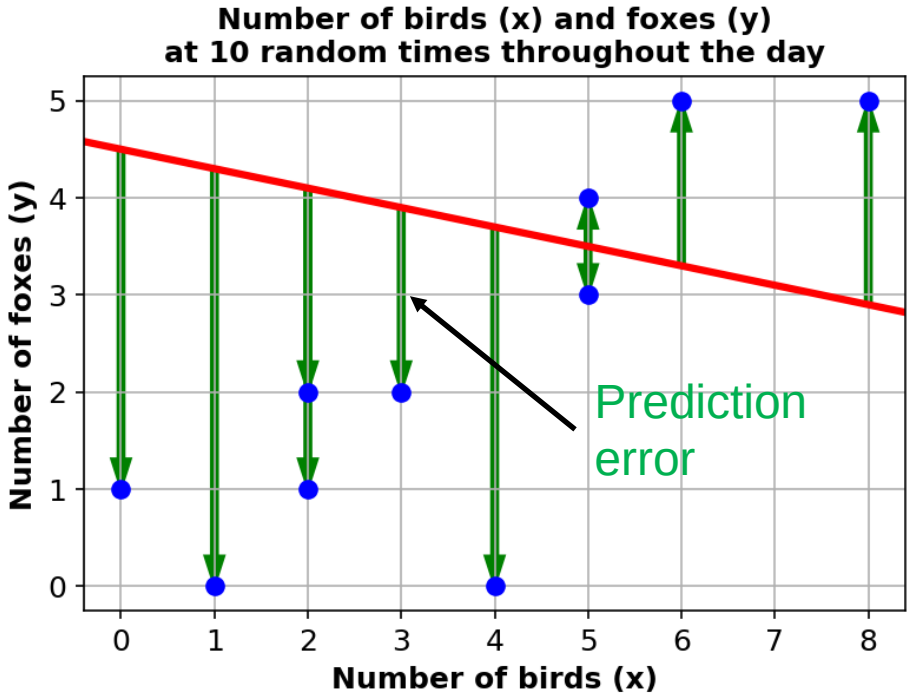


Training procedure

- **Weights initialization: Start with reasonable (or random) values for the model's weights:**
  m = -0.2 b = 4.5
- **Select a loss (or cost) function *L*(m, b) that describes how well the model fits the data with particular values of the weights**
- **Mean squared error:**

$$L(\mathrm{m}, \mathrm{b}) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - y_{i,\mathrm{predict}}(\mathrm{m}, \mathrm{b})\right)^2$$

- **Example calculation:**

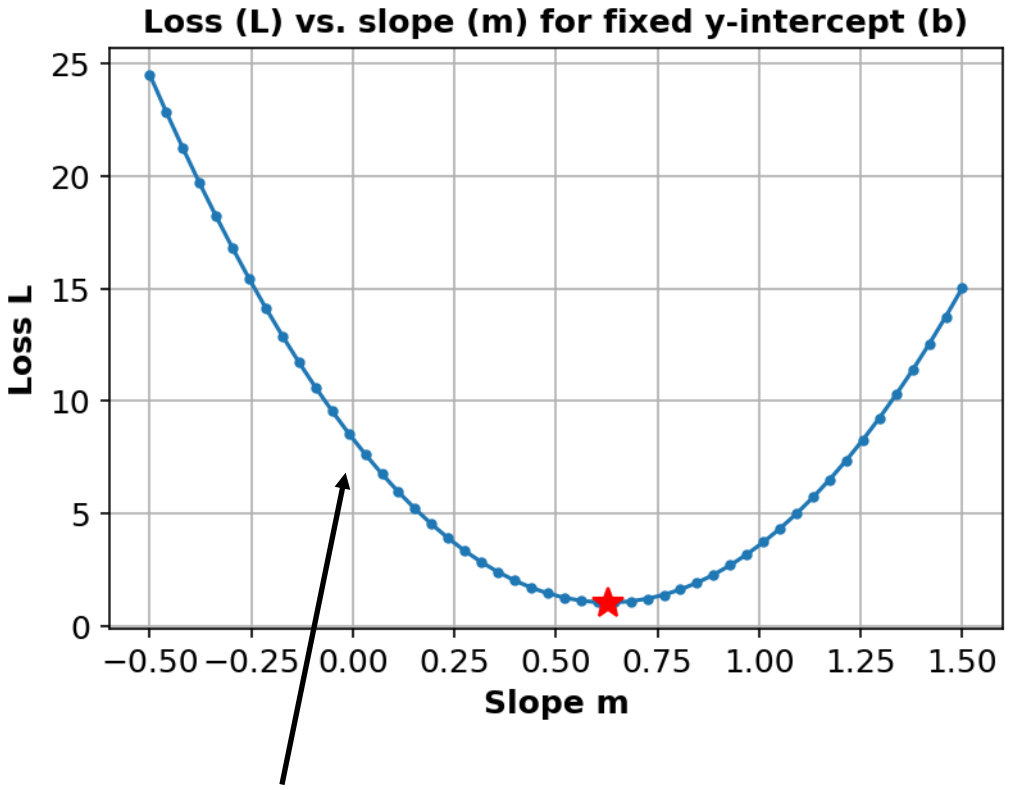


Sample ID (*i*)	# birds (x_i)	# foxes (y_i)	$y_{i,\mathrm{predict}}$(-0.2, 4.5)	(y_i – $y_{i,\mathrm{predict}}$(-0.2, 4.5))^2
1	5	3	3.5	0.25
2	2	2	4.1	4.41
⋮	⋮	⋮	⋮	⋮
N	5	4	3.5	0.25

Take average to obtain the starting loss:
L(-0.2, 4.5) = 6.99

Training procedure, ctd.

- **Point of training:** Minimize the loss *L*(m, b) by choosing better values for the weights m and b
- Weights are updated iteratively to reduce the loss
- A common algorithm for updating the weights is called gradient descent
- The model is said to be converged when the loss is minimized with respect to the weights
- This signifies the end of the training procedure

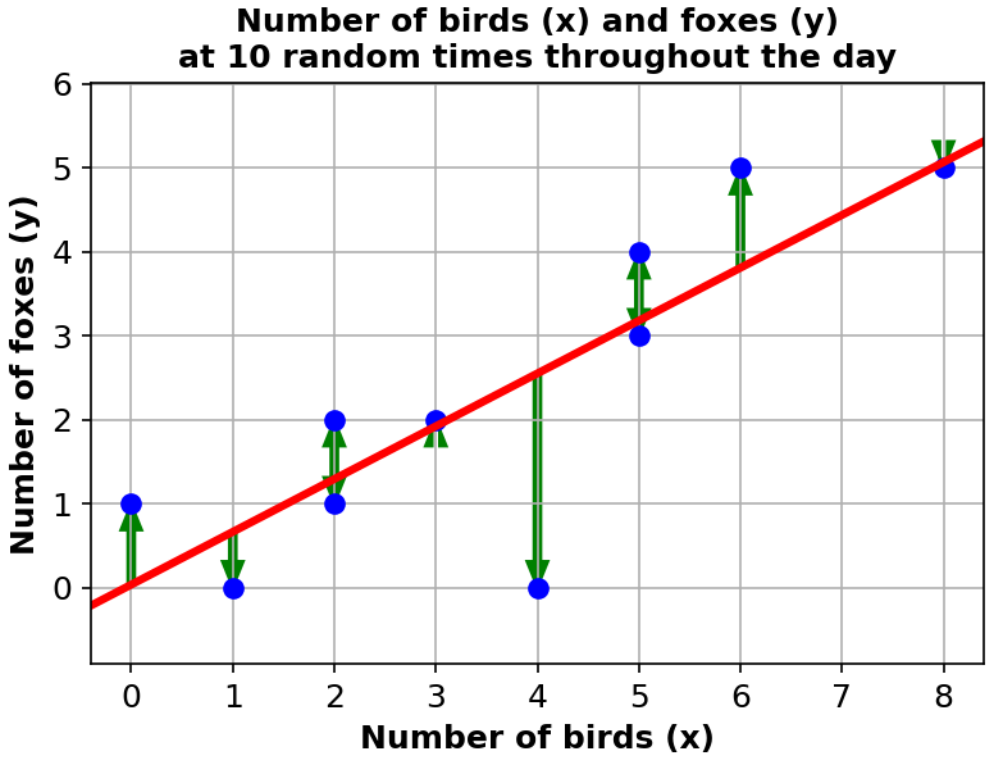


The degree the weights are allowed to change in an update step is called the learning rate

Training procedure: Key takeaways

- **After the training procedure is complete, you are left with weights (e.g., m and b) that allow you to most accurately predict the labels <u>using the selected model</u> (e.g., linear regression)**
- **In our example, we find**
  m = 0.63 b = 0.04
  are the weights that minimize the mean squared error, i.e., the loss
- **In other words, we are able to best predict the labels y_i in our training dataset using the formula:**

$$y_{i,\text{predict}}(0.63, 0.04) = 0.63x_i + 0.04$$



Testing procedure

- **Question: How does our model perform in the real world?**
  - We know our model performs as well as possible on the training dataset because that's what we used to optimize its weights
- **Answer: Provide some real-world data, called the testing dataset, that was not used for the training procedure**
  - Using the already-trained model (called inference), calculate the loss on the testing dataset, e.g.,

$$L_{\text{test}}(\mathbf{0.63}, \mathbf{0.04}) = \frac{\mathbf{1}}{N_{\text{test}}} \sum_{j=1}^{N_{\text{test}}} \left(\boldsymbol{y}_j - \boldsymbol{y}_{j,\mathbf{predict}}(\mathbf{0.63}, \mathbf{0.04}) \right)^{\mathbf{2}}$$

- **Using a holdout dataset such as a testing dataset helps to avoid overfitting the model to the training dataset**
- **This procedure gives you an idea of how well the model will generalize, informing you of the generalization error**

Data splitting

- **Data splitting is the process of splitting the available dataset into a training dataset and a testing dataset**
- **It is often as easy as taking a 70-30 or 80-20 split of the full dataset**
- **However, quality control measures must be taken to ensure both the training and testing datasets are representative of the real-world population**
- **Data splitting can include splitting into another dataset that is not used for training (other than the testing dataset) called the validation dataset**
- **The validation dataset is generally used for optimizing a model's hyperparameters**

	Number of birds (*x*)	Number of foxes (*y*)
Training dataset	5	3
	2	2
	1	0
	3	2
	6	5
	0	1
	4	0
Testing dataset	2	1
	8	5
	5	4

Hyperparameters

- A hyperparameter is a parameter that defines the model architecture itself
- It is not optimized in the training process
- For example, let's replace our linear regression model with a more-general polynomial regression model that we define as:

  $$y_{\text{predict}}(\{\theta\}) = \sum_{k=0}^{D} \theta_k x^k$$

  where *D* is the Degree of the polynomial
  - E.g., *D*=0: $y_{\text{predict}}(\theta_0) = \theta_0$
  - E.g., *D*=1: $y_{\text{predict}}(\theta_0, \theta_1) = \theta_0 + \theta_1 x$
  - E.g., *D*=2: $y_{\text{predict}}(\theta_0, \theta_1, \theta_2) = \theta_0 + \theta_1 x + \theta_2 x^2$
- We can say *D* is a hyperparameter of the polynomial regression model
- *D* defines the model architecture, including the weights $\{\theta\}$ that are present in the model
- Once *D* is specified and fixed, the weights are optimized as usual to minimize the loss

Hyperparameter optimization

- **Hyperparameter optimization is the process of optimizing a model's hyperparameters**
- **Just as you should evaluate a model's real-world performance on data that was not used in the training process (i.e., on a testing dataset)…**
  - …you should evaluate the effect of the hyperparameter values on data that was not used in the training process, on a third dataset called the validation dataset
- **Just as earlier we calculated L_{test} on the testing dataset using the already-trained model…**
  - …now we calculate L_{valid} on the validation dataset using the already-trained model
- **Note there are alternatives to "holding out" data just for validation, e.g., in cross-validation**

	Number of birds (*x*)	Number of foxes (*y*)
Training dataset	5	3
	2	2
	1	0
	3	2
	6	5
Validation dataset	0	1
	4	0
Testing dataset	2	1
	8	5
	5	4

Sample workflow for the polynomial regression model

- **For the *D*=0 model, optimize the weight θ_0 on the training dataset**
  - Evaluate the resulting model on the validation dataset, i.e., calculate $L_{\text{valid}}(D = 0)$
- **For the *D*=1 model, optimize the weights $\{\theta_0, \theta_1\}$ on the training dataset**
  - Evaluate the resulting model on the validation dataset, i.e., calculate $L_{\text{valid}}(D = 1)$
- **For the *D*=2 model, optimize the weights $\{\theta_0, \theta_1, \theta_2\}$ on the training dataset**
  - Evaluate the resulting model on the validation dataset, i.e., calculate $L_{\text{valid}}(D = 2)$
- **Etc. for $D \geq 3$**
- **Choose the value of *D* for which $L_{\text{valid}}(D)$ is a minimum**
  - Congratulations, you have just optimized the hyperparameter *D*!
- **Train the corresponding model on the training+validation datasets**
  - This yields your best model
- **Evaluate this model on the test dataset, i.e., calculate L_{test}**
  - This is your estimate of the generalization error

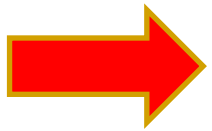
	Number of birds (*x*)	Number of foxes (*y*)
Training dataset	5	3
	2	2
	1	0
	3	2
	6	5
Validation dataset	0	1
	4	0
Testing dataset	2	1
	8	5
	5	4

Increasing the number of features

Number of birds (x)	Number of foxes (y)
5	3
2	2
1	0
3	2
6	5
0	1
4	0
2	1
8	5
5	4

x y

vector



Number of birds (x_1)	Number of cicadas (x_2)	Number of foxes (y)
5	90	3
2	30	2
1	50	0
3	50	2
6	40	5
0	20	1
4	70	0
2	40	1
8	150	5
5	30	4

X y

matrix

Data for classification tasks

Image classification

Image ID	Pixel 1	Pixel 2	. . .	Pixel *M*	Class
1	155	42	⋯	210	Hot dog (1)
2	24	255	⋯	192	Hot dog (1)
⋮	0	137	⋯	5	Not hot dog (0)
N	1	2	⋯	35	Hot dog (1)
		X			***y***

Cancer type classification using RNA-Seq counts data

Sample ID	Gene 1	Gene 2	. . .	Gene *M*	Cancer type
1	12005	2	⋯	500	Liver (0)
2	20000	500	⋯	1005	Pancreatic (1)
⋮	8888	0	⋯	459	Liver (0)
N	9000	5	⋯	1208	Breast (2)
		X			***y***

Supervised learning summary

- **In supervised learning, you generally start with a feature matrix *X* and a labels vector *y***
- **Select a model, which will contain adjustable weights $\{\theta\}$**
- **Train the model on *X* and *y* by minimizing a loss with respect to the weights $\{\theta\}$**
- **Then, obtain a single new sample, e.g.:**
  - Number of birds
  - Number of birds and number of cicadas
  - An image
  - RNA-Seq counts data from a single biological sample
- **Input this sample into the trained model (i.e., in inference mode) in order to make a prediction, e.g.:**
  - Number of foxes
  - Hot dog or not hot dog
  - Tumor type

Supervised learning summary, ctd.

- **In addition to making a prediction, some models are able to explain why that prediction was made**
  - This generally means informing the user which features were most crucial to making predictions
  - This is called feature importance
  - For example:
    - Were the number of birds more important than the number of cicadas in determining the number of foxes?
    - Which pixels in the image were most important in determining whether the image was a hot dog?
    - Which genes are most important in determining the type of tumor?
- **Often, the more complex the model, the harder it is to explain its predictions**
- **Sample supervised learning models: linear/polynomial regression, logistic regression, K-nearest neighbors, perceptron, support vector machines, random forests, neural networks**

Aside: Deep learning

- **When a reasonably large neural network model is used for a machine learning task, deep learning is being performed**
- **Deep learning is just a subset of machine learning**
- **It is special because the model architecture and the algorithms used to update its weights fit perfectly on graphics processing units (GPUs)**
  - I.e., we already have hardware specialized for deep learning!
- **As neural networks are often very large, they are also very powerful**
  - Major application in intensive tasks such as facial recognition and word/phrase prediction

Unsupervised learning

- **In unsupervised learning, the labels *y* are not provided (nor is there a need for them)**
- **Instead of prediction, the goal is to learn about the feature matrix *X* itself**
- **Sample questions that are asked:**
  - Which samples are similar to each other (clustering), or which ones are outliers?
  - Can we reduce the number of features to a smaller set of better-discriminating features (dimensionality reduction)?
- **Just as in supervised learning, these methods generally optimize weights to minimize a cost function**
- **Sample unsupervised learning models: K-Means, Gaussian mixture models, principal component analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), autoencoders**

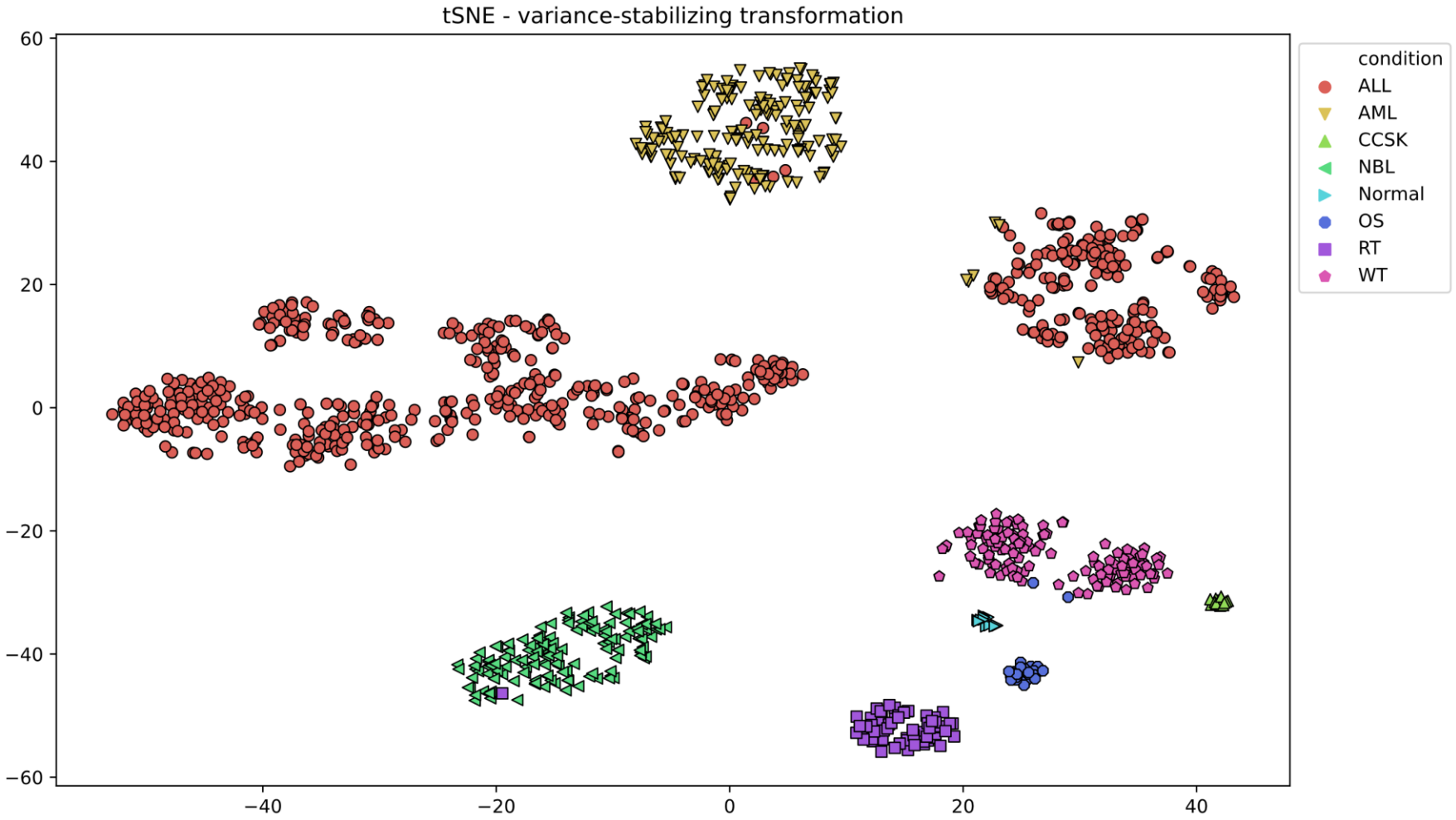
Example of dimensionality reduction on RNA-Seq counts data

- **Recall format of the data:**

Sample ID	Gene 1	Gene 2	. . .	Gene *M*	Cancer type
1	12005	2	⋯	500	Liver (0)
2	20000	500	⋯	1005	Pancreatic (1)
⋮	8888	0	⋯	459	Liver (0)
N	9000	5	⋯	1208	Breast (2)
			X		***y***

- **Reduce the dimensionality of the feature matrix *X* using t-SNE**
- **Create a scatterplot of the two most highly varying, transformed features**
- **Color the datapoints by their labels *y***

Example of dimensionality reduction on RNA-Seq counts data, ctd.



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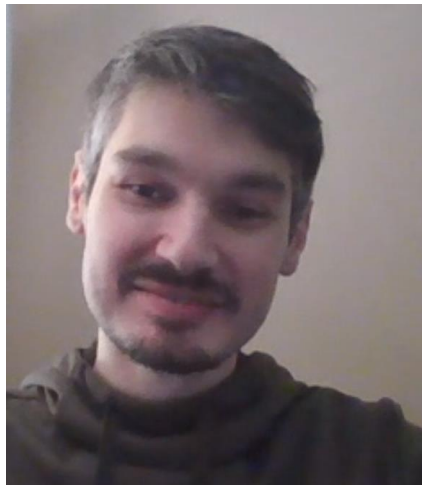

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Questions?