Supervised Learning

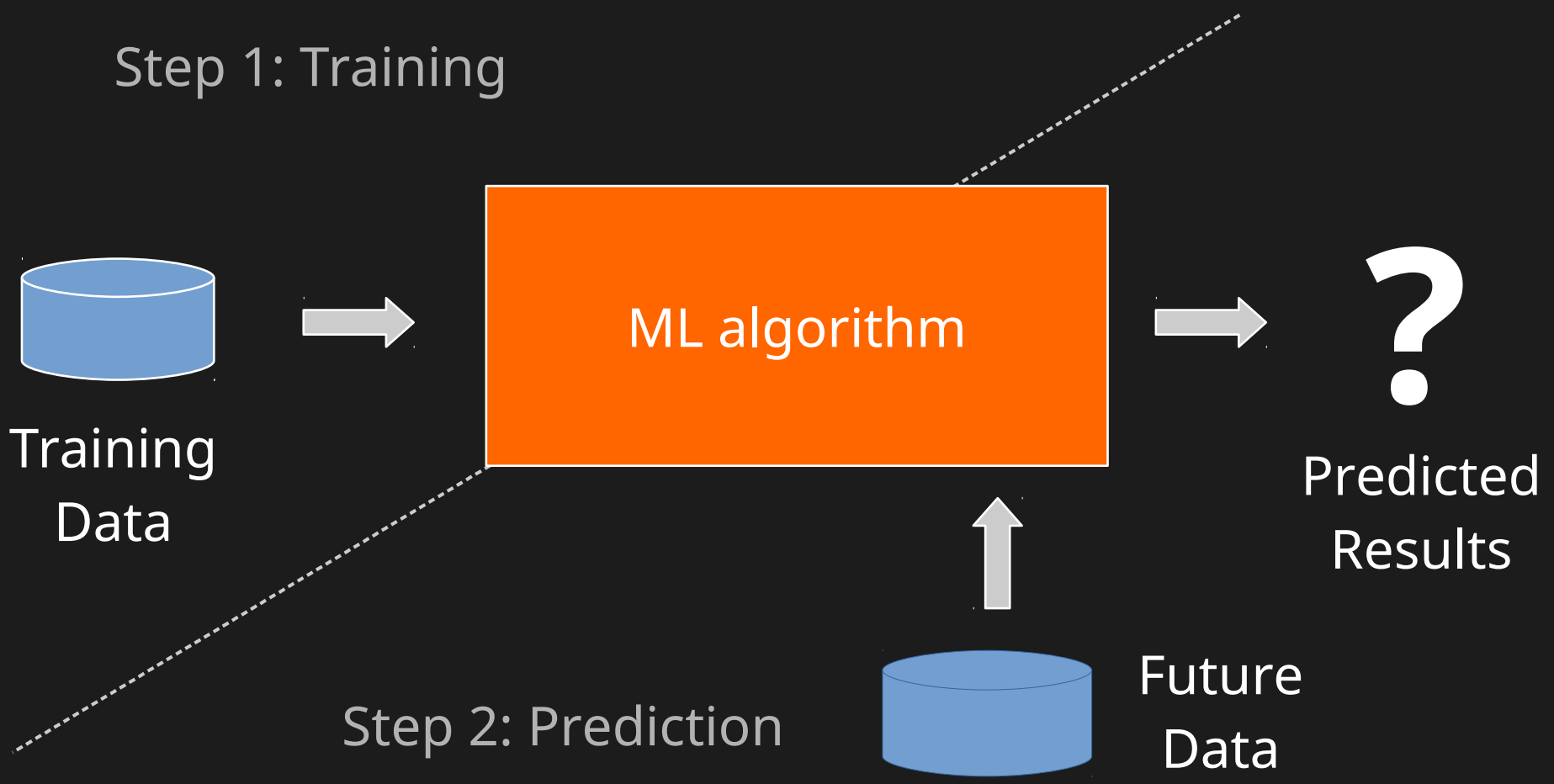
Concepts

Reminder: Supervised Learning

- Let the computer learn a task by providing (a lot of) examples

- Main applications:
  - Regression: predict a continuous variable
  - Classification: predict class affiliation

How does it work?



Stationary assumption:
training and future data are independent and identically distributed (i.i.d.)

Data: Nomenclature

Features (input variables)

Targets/Labels (output variables)

Examples

Weight	Height	Exterior	Wings?	Lika-bility	N_{legs}	Pet?	Type
0.1	0.1	feath.	true	1	2	true	bird
3.5	0.3	fur	false	1	4	true	cat
12.0	0.7	fur	false	1	4	true	dog
500	1.8	skin	false	2	4	false	rhinoceros
800	3.0	fur	true	3	4	false	chimera
2.5	0.5	fur	false	1	4	true	cat
...	...	...	...	...	...	...	...

classes of label "Type"

Data Type:

continuous	continuous	categorical	binary	ordinal	integer	binary	categorical (multi-class)

Data Preparation

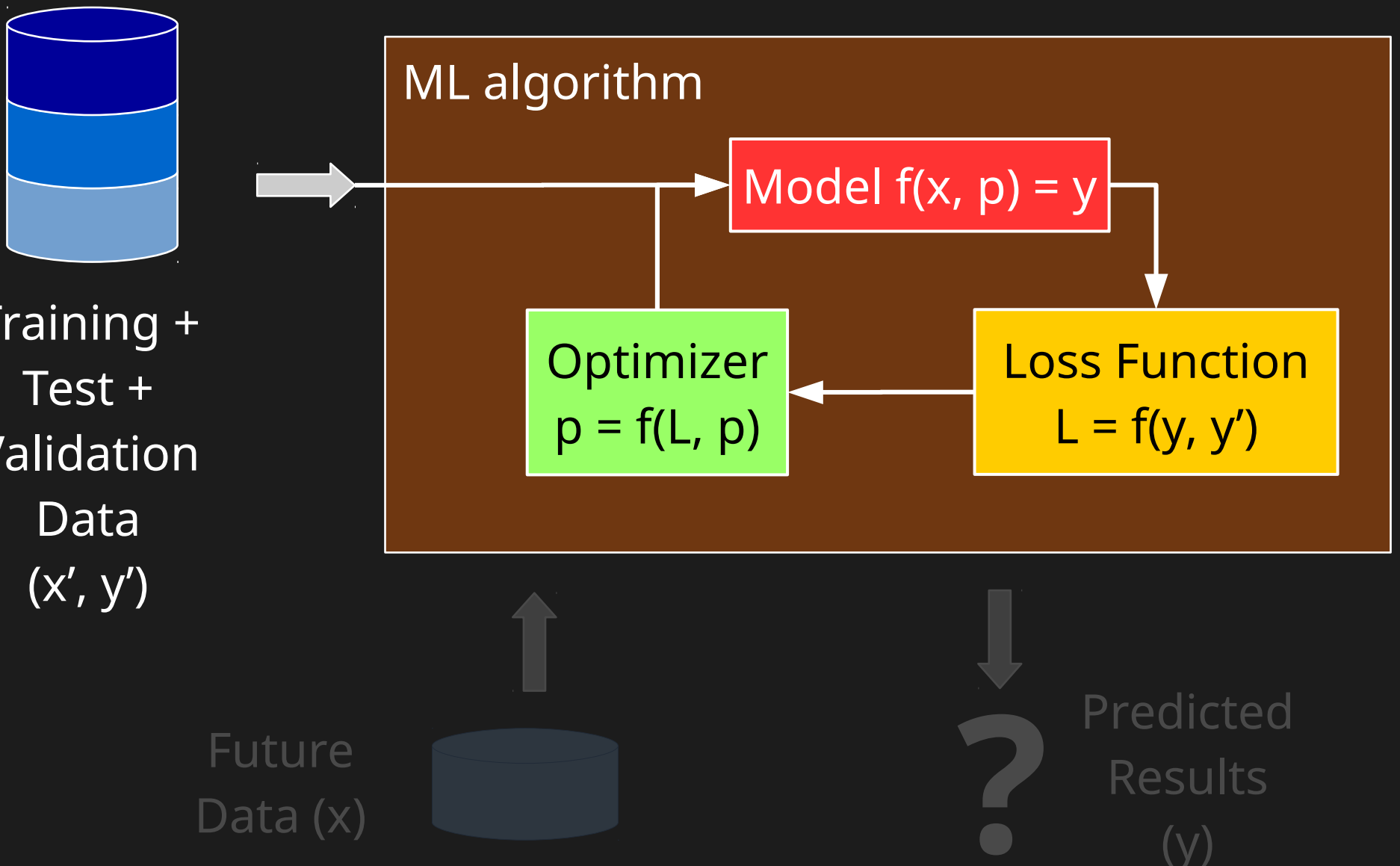
- Keep in mind that not all data can be handled easily by machines:
  - **Continuous data** (floats, integers): fine!
  - **Categorical data**: nope.
    → one-hot encoding
  - **Binary data**: fine, but has to be numerical
  - **Ordinal data**: fine, but has to be numerical
- One-hot encoding can exponentially raise the number of features in your data set

Data Samples

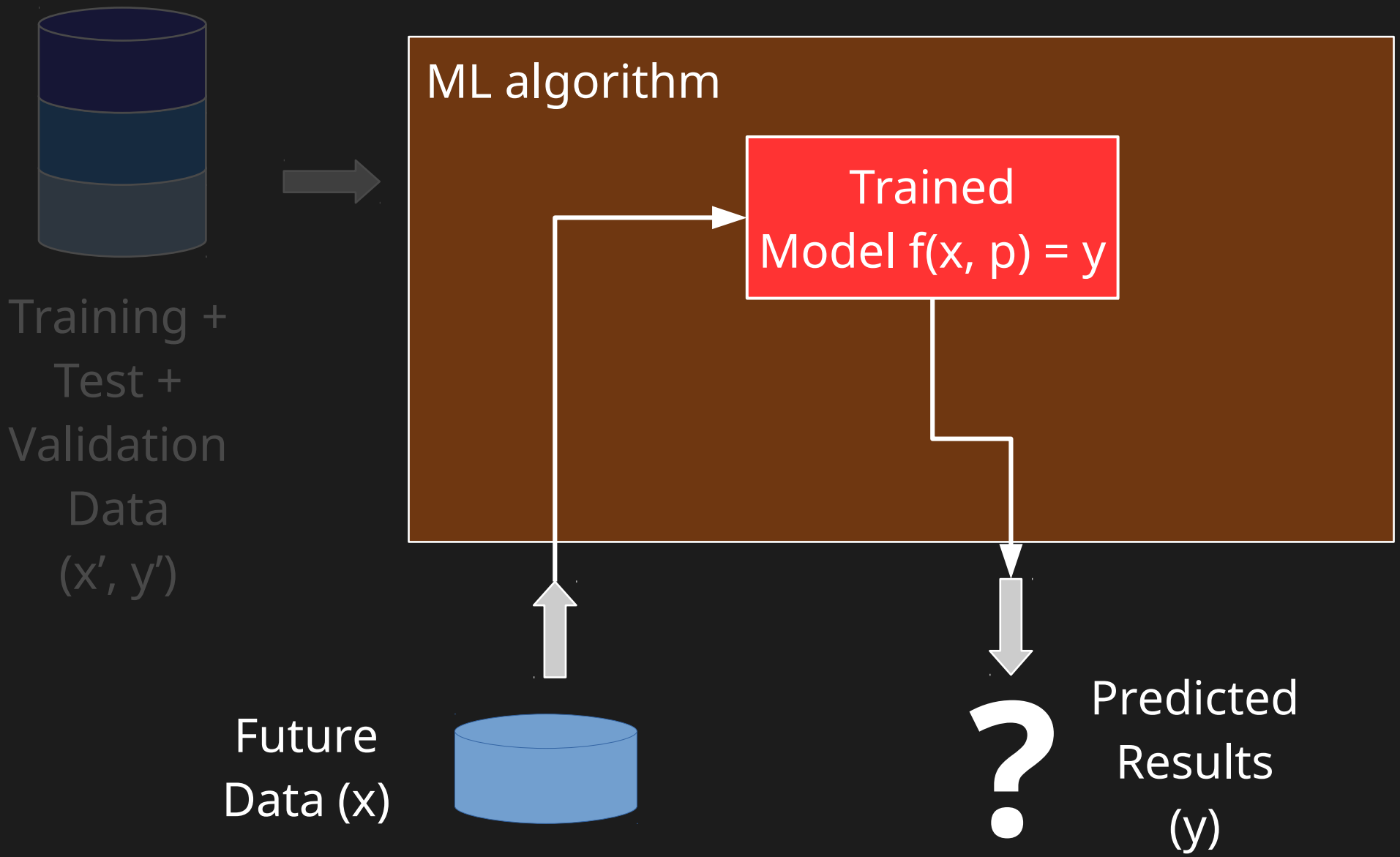
- **Training data**: features + labels
  used as examples for training the ML model
- **Test data**: features + labels
  used for evaluating the accuracy of the trained model; must be different from training data
- **Validation data**: features + labels
  used for validating the model settings
- **Future data**: features
  used to evaluate model and predict labels

- All data must be i.i.d.!

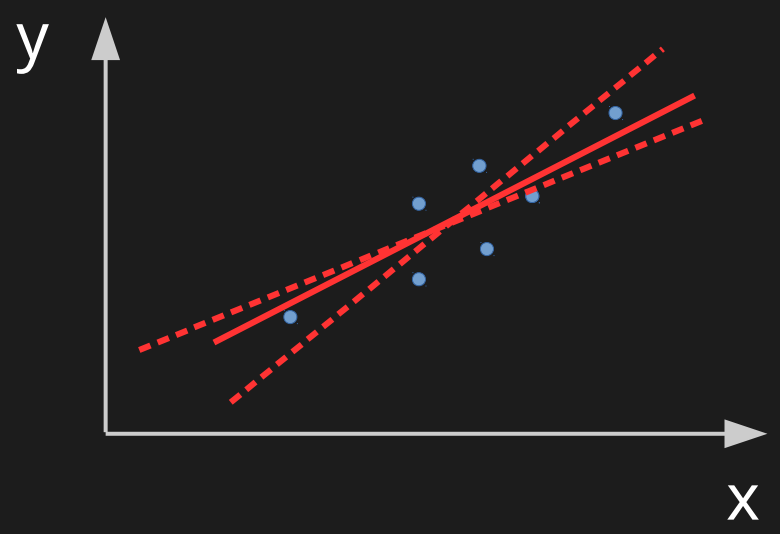
How does Supervised Learning work? Learning Stage:



How does Supervised Learning work? Prediction Stage:



Linear Regression as ML Example



Training Data $\{(x_1', y_1'), (x_2', y_2'), \ldots\}$

Model $f(x_i, \vec{p}) = p_0 + p_1 \cdot x_i$

Parameters/ Weights $\vec{p} = (p_0 \; p_1)^T$

How do we fit the model to the data?

Loss Function $L(\vec{x}, \vec{y}') = \sum_i [f(x_i) - y_i']^2$

Optimizer: $\frac{\partial L}{\partial \vec{p}} = \vec{0}$ → $\vec{p}$

Loss Functions and Metrics

- Loss/Objective functions calculate loss
- Loss is used to improve the model parameters

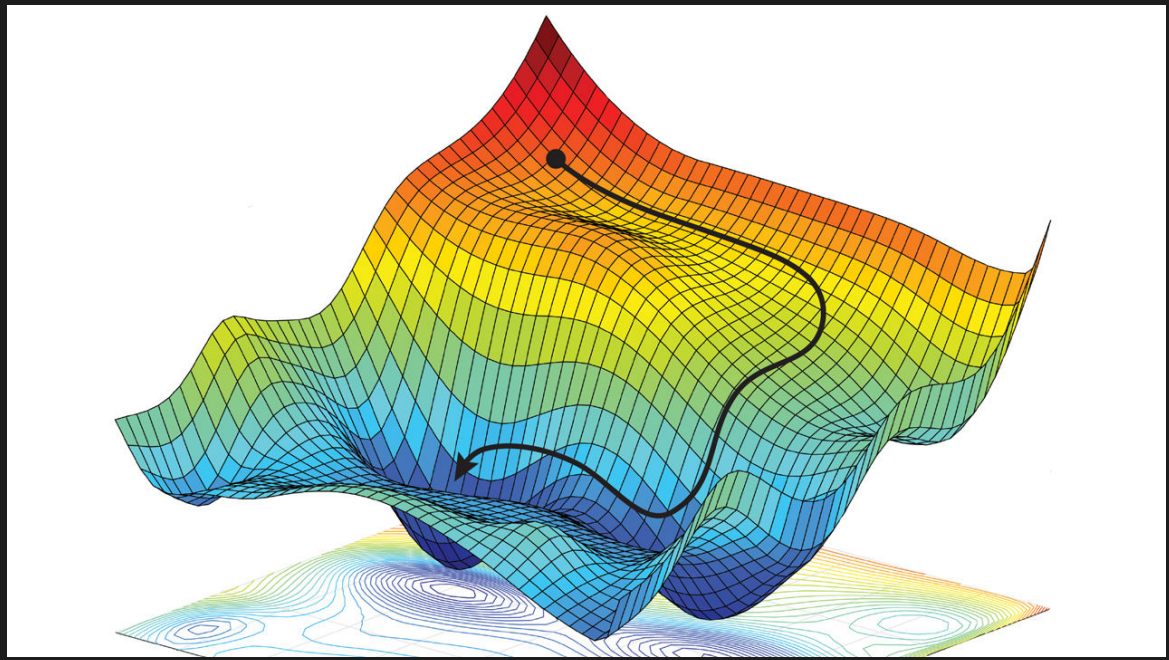
- Metrics benchmark the model's success (**score**) examples:
  - Accuracy (classification): $N_{correct}/N_{total}$
  - Root-Mean-Square-Error (regression)

- Regression metrics may be used as loss functions, but generally they are two different things

Optimizers

- In the case of linear regression, you can immediately solve for the best-fit parameters
- More complex (non-linear) models and loss functions require an iterative approach
- All-round optimizer: gradient descent

$$\vec{p}_{i+1} = \vec{p}_i - \alpha \nabla_p L(y, y')$$



Classification: Balance and Errors

- Accuracy is a simple metric, but can be misleading:

  “1 in 1000 emails is spam.”

  By assuming no email is spam you get a 99.9% accuracy. But that’s not the idea…

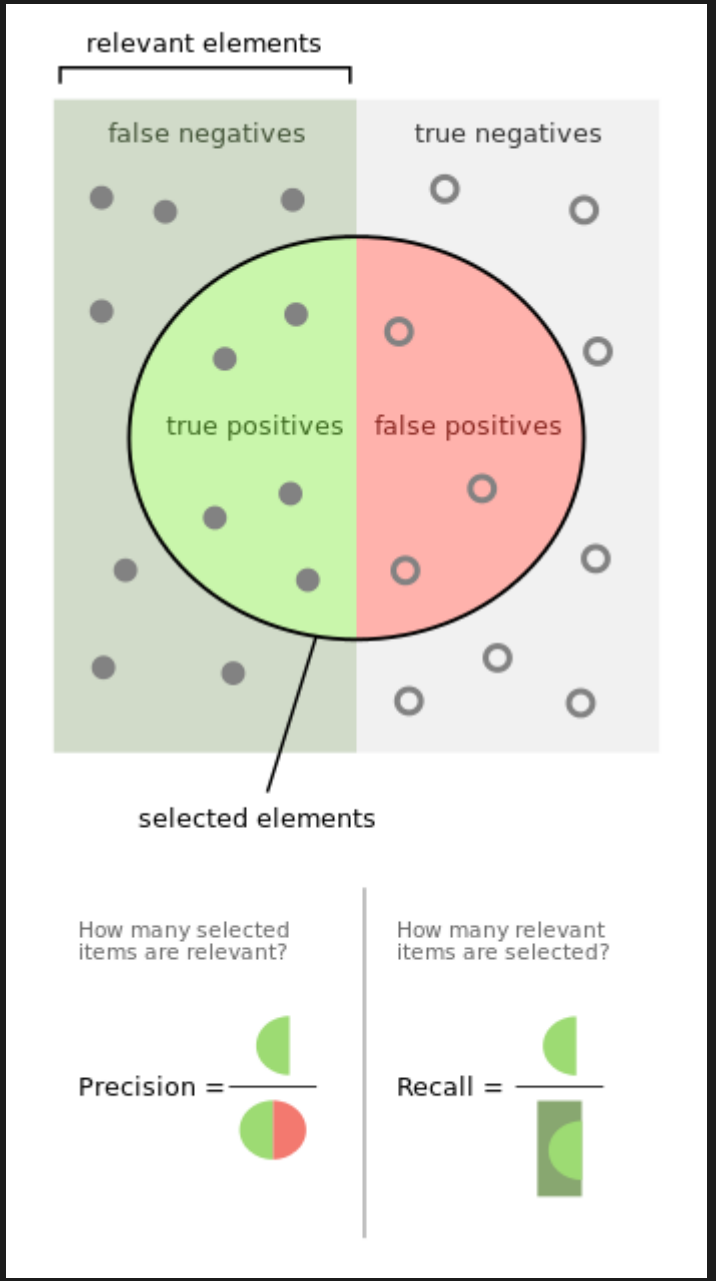
- Accuracy is a bad metric if the data set (i.e., their classes) is unbalanced
- Have to account for application and different errors...

Classification: Balance and Errors

- Precision and Recall can be better metrics - depending on application:
  - spam filter: max precision
  - cancer diagnosis: max recall

- Good compromise:

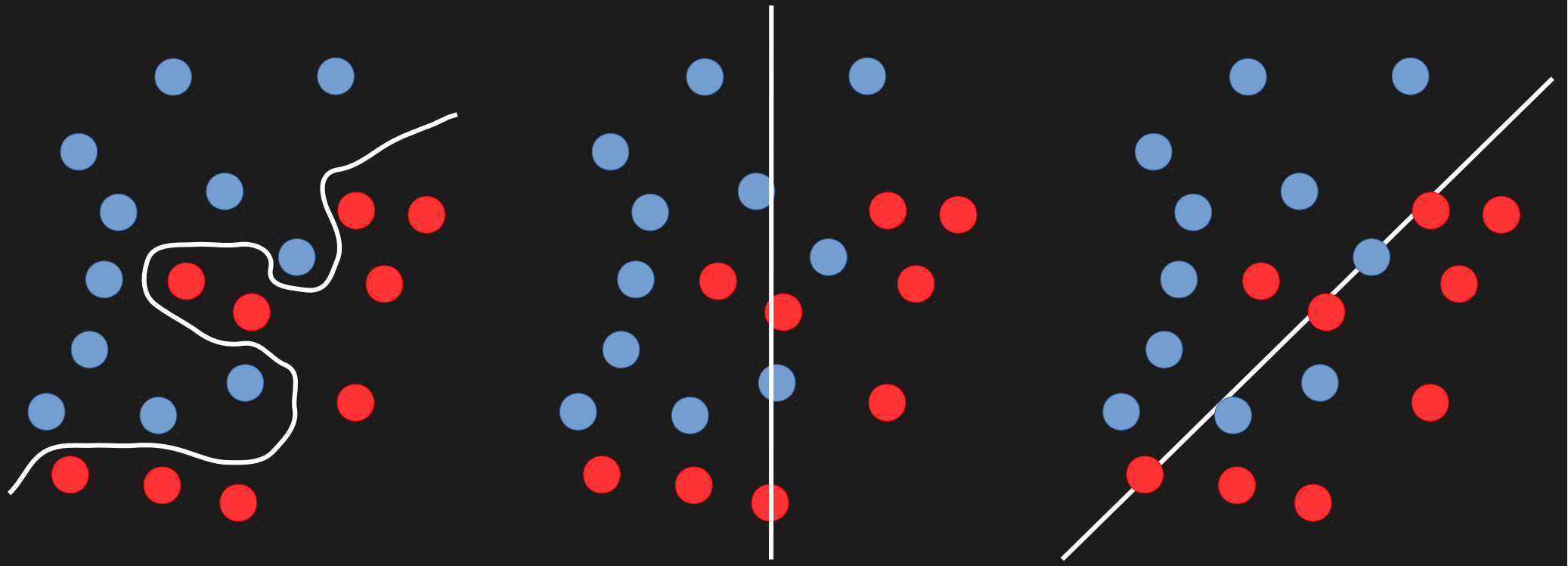
$$F1 = 2 * \frac{(Precision * Recall)}{(Precision + Recall)}$$



wikipedia

Generalization

- What if you get a high training score, but a low test/validation sample score?



Low Generalization
Overfitting

High Generalization
Underfitting

Good Generalization
Good fit

Generalization and Regularization

- Overfitting: high training score, low test score
- Good fit: similar training and test scores
- Underfitting: low training and test scores

- Generalization can be enforced through regularization as part of the training process by imposing a penalty on the loss function (more on the details later)

Cross-Validation

- Data is typically expensive
- But we need training/test/validation data, all of which have to be exclusive samples

- We can recycle data!

1. Shuffle

2. Split

3. Train model and get scores

4. redo N times and pick best/mean score

Hyperparameters

- Hyperparameters are model parameters that are not learned; they are set by the user
- Hyperparameters need tuning by the user
- Expensive: run a full-blown training with different hyperparameter settings
- sklearn: gridsearchcv combines a gridsearch over hyperparameters with cross-validation

General Approach

- Prepare the data: Identify and format the features and targets, scale data
- Pick a suitable model: regression/classification, complexity
- Train the model (training + test data)
- Tune hyperparameters
- Check model performance (validation data)
- Predict future data

sklearn

- sklearn has implementations of most standard models available
- Training and hyperparameter tuning can be automated using gridsearchcv and pipelines
- More complex third-party models (e.g., lightgbm) often provide interfaces to the sklearn infrastructure and can be used like sklearn models
- More about this next time...