Active Learning

CS 203: Software Tools and Techniques for AI

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The Labeling Problem

Scenario: You need to train a classifier

Traditional approach:

1. Collect 10,000 images
2. Label all 10,000 images
3. Train model
4. Hope it works

The cost:

- 10,000 labels × 30 seconds = 83 hours
- At $20/hour = $1,660
- Many labels are redundant

What is Active Learning?

Active Learning: Intelligently select which examples to label to maximize model performance with minimal labeling effort

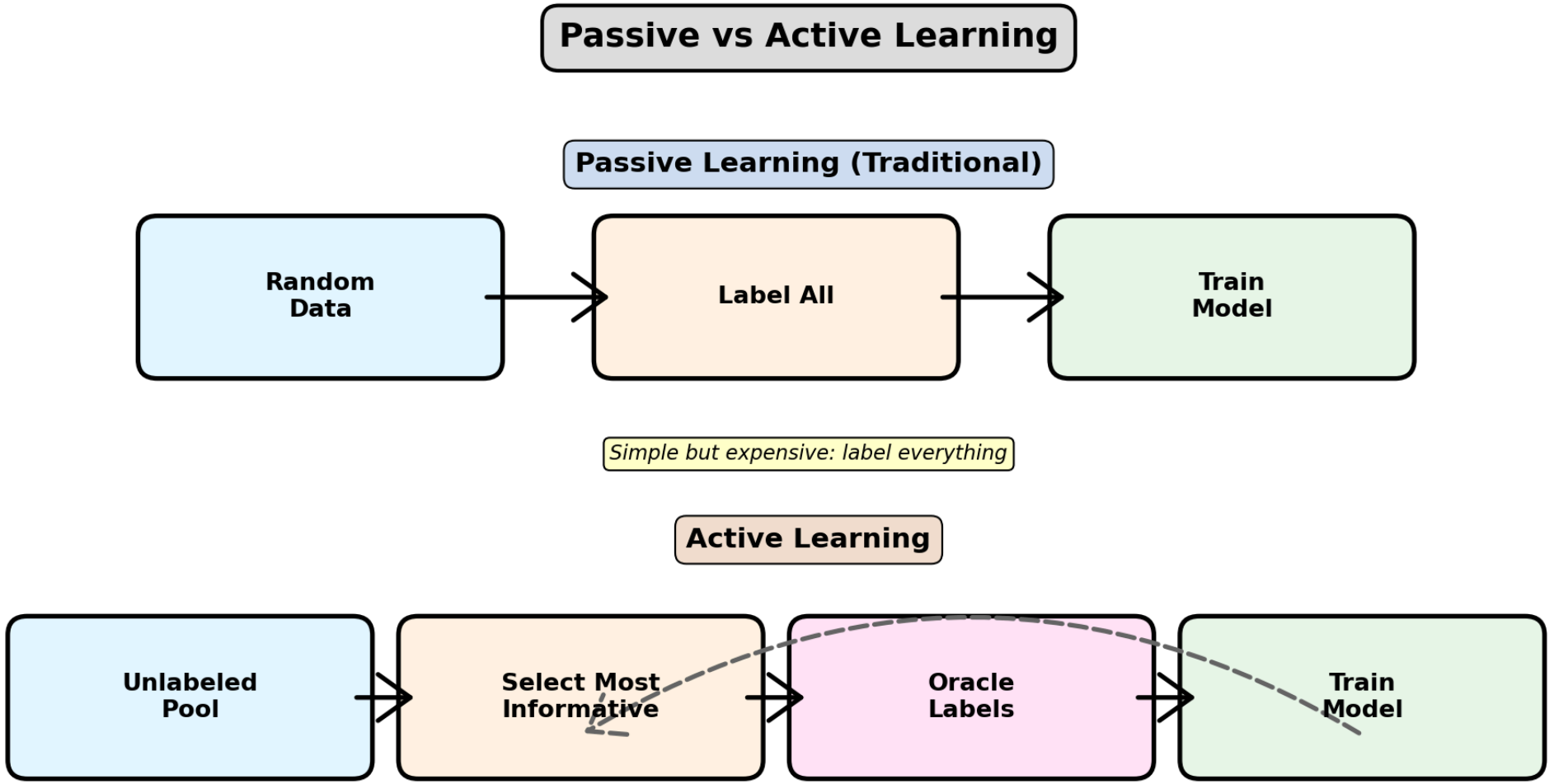
Key Insight: Not all data points are equally valuable for learning!

Example:

- 100 random samples might give 85% accuracy
- 100 carefully chosen samples might give 92% accuracy

Goal: Achieve same performance with 5-10× fewer labels

Passive vs Active Learning



When to Use Active Learning

Use Active Learning when:

- Labeling is expensive (human time, expert knowledge)
- You have large unlabeled dataset
- You need good performance with limited labels
- Labels are imbalanced or rare

Real-world applications:

- Medical imaging (radiologist time is expensive)
- Legal document review (lawyer expertise)
- Rare event detection (fraud, defects)
- Custom domain classification

Active Learning Cycle

The Loop:

1. **Start**: Train initial model on small labeled set
2. **Query**: Select most informative unlabeled examples
3. **Oracle**: Human labels selected examples
4. **Update**: Retrain model with new labels
5. **Repeat**: Until performance target or budget reached

Key components:

- **Learner**: ML model being trained
- **Query Strategy**: How to select examples
- **Oracle**: Human labeler (or simulation)

Query Strategies: Comparison

Strategy	Approach	Pros	Cons	Best For
Uncertainty Sampling	Pick most uncertain examples	Simple, fast, effective	May cluster in decision boundary	Most tasks (default choice)
Query-by-Committee	Pick where models disagree	Robust, diverse	Requires training multiple models	When you can afford ensembles
Expected Model Change	Pick examples that change model most	Adaptive	Computationally expensive	When labels are very expensive
Diversity	Pick diverse	Covers	Ignores model	Imbalanced or

Uncertainty Sampling

Idea: Label examples where the model is most confused

For binary classification:

- Model predicts P(positive) = 0.51
- Model is uncertain! Label this example

For multi-class:

- Model predicts [0.34, 0.33, 0.33]
- Very uncertain! Label this

Intuition: Easy examples don't teach us much. Hard examples are informative.

Uncertainty Measures: Mathematical Foundation

Problem Setup

Given:

- Model f with parameters θ
- Unlabeled example x
- Class predictions $P_\theta(y|x)$ for classes $y \in \{1, \ldots, C\}$

Goal: Define uncertainty $U(x)$ to select most informative examples

Uncertainty Measure 1: Least Confident

Formula

$$U_{LC}(x) = 1 - P_\theta(\hat{y}|x)$$

where $\hat{y} = \arg\max_y P_\theta(y|x)$ is the predicted class

Interpretation

- Measures how uncertain the model is about its top prediction
- Range: [0, 1]
- High value = low confidence = select for labeling

Example

Probabilities: $P(y|x) = [0.6, 0.3, 0.1]$

Uncertainty Measure 2: Margin Sampling

Formula

$$U_M(x) = P_\theta(\hat{y}_1|x) - P_\theta(\hat{y}_2|x)$$

where:

- $\hat{y}_1$ = most probable class
- $\hat{y}_2$ = second most probable class

Then uncertainty is:

$$U_M^{inv}(x) = 1 - U_M(x)$$

Interpretation

- Small margin = model is confused between top 2 classes

Margin Sampling: Example

Scenario

Example A: $P(y|x) = [0.51, 0.49, 0.00]$

$$U_M(A) = 0.51 - 0.49 = 0.02 \quad (\text{very small margin})$$

Example B: $P(y|x) = [0.99, 0.01, 0.00]$

$$U_M(B) = 0.99 - 0.01 = 0.98 \quad (\text{large margin})$$

Selection: Example A is more uncertain → select for labeling

Comparison with Least Confident:

- $U_{LC}(A) = 1 - 0.51 = 0.49$
- $U_{LC}(B) = 1 - 0.99 = 0.01$

Both correctly identify A as more uncertain!

Uncertainty Measure 3: Entropy

Formula

$$H(P_\theta(y|x)) = -\sum_{y=1}^{C} P_\theta(y|x) \log P_\theta(y|x)$$

Interpretation

- Measures disorder/uncertainty in probability distribution
- Range: $[0, \log C]$
- Maximum when all classes equally likely
- Most theoretically principled measure

Properties

Entropy: Detailed Example

Binary Classification ($C = 2$)

Example 1 (very confident):

$$P(y|x) = [0.95, 0.05]$$

$$H = -0.95 \log(0.95) - 0.05 \log(0.05) = 0.286$$

Example 2 (uncertain):

$$P(y|x) = [0.5, 0.5]$$

$$H = -0.5 \log(0.5) - 0.5 \log(0.5) = 0.693$$

Maximum possible: $\log(2) = 0.693$

Selection: Example 2 has higher entropy → more uncertain

Entropy: Multi-Class Example

3-Class Classification ($C = 3$)

Example A (confident):

$$P(y|x) = [0.8, 0.15, 0.05]$$

$$H_A = -(0.8 \log 0.8 + 0.15 \log 0.15 + 0.05 \log 0.05) = 0.849$$

Example B (uncertain):

$$P(y|x) = [0.4, 0.35, 0.25]$$

$$H_B = -(0.4 \log 0.4 + 0.35 \log 0.35 + 0.25 \log 0.25) = 1.571$$

Example C (maximum uncertainty):

$$P(y|x) = [0.33, 0.33, 0.33]$$

$$H_C = -3 \times (0.33 \log 0.33) = 1.585 \approx \log(3) = 1.099$$

Comparing Uncertainty Measures

Measure	Formula	Best For	Limitations
Least Confident	$1 - \max_y P(y\|x)$	Simple, fast	Ignores distribution shape
Margin	$P(\hat{y}_1\|x) - P(\hat{y}_2\|x)$	Binary/multiclass	Only considers top 2
Entropy	$-\sum_y P(y\|x) \log P(y\|x)$	Full distribution	More computation

Example Comparison

$P(y|x) = [0.6, 0.3, 0.05, 0.05]$

- Least Confident: $U = 0.4$
- Margin: $U = 0.3$
- Entropy: $U = 1.23$

Uncertainty Sampling - Code

Uncertainty Sampling - Code

Basic implementation:

```
from sklearn.linear_model import LogisticRegression
import numpy as np

def uncertainty_sampling(model, X_unlabeled, n_samples=10):
    # Get prediction probabilities
    probs = model.predict_proba(X_unlabeled)

    # Calculate uncertainty (1 - max probability)
    uncertainties = 1 - np.max(probs, axis=1)

    # Select top uncertain samples
    indices = np.argsort(uncertainties)[-n_samples:]

    return indices

# Usage
```

Query-by-Committee: Mathematical Foundation

Setup

Committee: $\mathcal{C} = \{h_1, h_2, \ldots, h_M\}$ of M models

- Each h_i trained on same labeled data $\mathcal{L}$
- Different algorithms or random initializations

For unlabeled example x:

- Get prediction distribution from each model: $P_{h_i}(y|x)$

Goal: Measure disagreement among committee members

QBC Disagreement Measure 1: Vote Entropy

Formula

$$D_{VE}(x) = -\sum_{y=1}^{C} \frac{V(y)}{M} \log \frac{V(y)}{M}$$

where $V(y)$ = number of committee members voting for class y

Example

Committee of 5 models, binary classification:

- 3 models predict class 0
- 2 models predict class 1

$$V(0) = 3, \quad V(1) = 2$$

QBC Disagreement Measure 2: Consensus Entropy

Formula

Average prediction distribution across committee:

$$P_C(y|x) = \frac{1}{M} \sum_{i=1}^{M} P_{h_i}(y|x)$$

Then calculate entropy of consensus:

$$D_{CE}(x) = H(P_C(y|x)) = -\sum_{y=1}^{C} P_C(y|x) \log P_C(y|x)$$

Interpretation

- Uses full probability distributions, not just votes

QBC: Detailed Example

Scenario: 3 Models, Binary Classification

	$P(y=0\|x)$	$P(y=1\|x)$
Model 1	0.9	0.1
Model 2	0.4	0.6
Model 3	0.3	0.7

Calculate Consensus Distribution

$$P_C(y=0|x) = \frac{0.9 + 0.4 + 0.3}{3} = 0.533$$

$$P_C(y=1|x) = \frac{0.1 + 0.6 + 0.7}{3} = 0.467$$

QBC Disagreement Measure 3: KL Divergence

Formula

Measure divergence of each model from consensus:

$$D_{KL}(x) = \frac{1}{M} \sum_{i=1}^{M} KL(P_{h_i}(y|x) \| P_C(y|x))$$

where KL divergence is:

$$KL(P \| Q) = \sum_{y} P(y) \log \frac{P(y)}{Q(y)}$$

Interpretation

- Measures how much individual predictions differ from average

KL Divergence: Example

Using previous example, consensus is $P_C = [0.533, 0.467]$

Model 1: $P_{h_1} = [0.9, 0.1]$

$$KL_1 = 0.9 \log \frac{0.9}{0.533} + 0.1 \log \frac{0.1}{0.467} = 0.397$$

Model 2: $P_{h_2} = [0.4, 0.6]$

$$KL_2 = 0.4 \log \frac{0.4}{0.533} + 0.6 \log \frac{0.6}{0.467} = 0.056$$

Model 3: $P_{h_3} = [0.3, 0.7]$

$$KL_3 = 0.3 \log \frac{0.3}{0.533} + 0.7 \log \frac{0.7}{0.467} = 0.130$$

Query-by-Committee - Code

Query-by-Committee - Code

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from scipy.stats import entropy

def query_by_committee(committee, X_unlabeled, n_samples=10):
    # Get predictions from all committee members
    all_probs = []
    for model in committee:
        probs = model.predict_proba(X_unlabeled)
        all_probs.append(probs)

    all_probs = np.array(all_probs)  # Shape: (n_models, n_samples, n_classes)

    # Calculate vote entropy for each sample
    avg_probs = all_probs.mean(axis=0)
    disagreements = entropy(avg_probs.T)

    # Select top disagreement samples
    indices = np.argsort(disagreements)[-n_samples:]
    return indices

# Create committee
committee = [
    RandomForestClassifier(),
    LogisticRegression(),
    SVC(probability=True)
]
```

Expected Model Change

Idea: Select examples that will change the model parameters most if labeled

Approach:

- For each unlabeled example, simulate adding it with each possible label
- Measure how much model parameters change
- Select examples causing largest change

Gradient-based:

```
# For each example x:
gradient = model.compute_gradient(x)
impact = ||gradient||  # Magnitude of gradient
```

Pros: Directly optimizes for model learning

Cons: Computationally expensive (need to retrain or compute gradients)

Diversity Sampling

Problem: Uncertainty sampling can select similar examples

Solution: Also consider diversity

Approaches:

1. **K-means clustering**: Select one example from each cluster
2. **Core-set selection**: Select examples that best represent all data
3. **Hybrid**: Combine uncertainty + diversity

```
from sklearn.cluster import KMeans

def diverse_uncertainty_sampling(model, X_unlabeled, n_samples=10):
    # First, get uncertain examples (2x more than needed)
    probs = model.predict_proba(X_unlabeled)
    uncertainties = 1 - np.max(probs, axis=1)
    uncertain_indices = np.argsort(uncertainties)[-n_samples*2:]
```

Cold Start Problem

Challenge: How to start with no labeled data?

Solutions:

1. **Random Sampling**: Label small random set to bootstrap

```
# Start with 20-50 random examples
initial_indices = np.random.choice(len(X_pool), size=20, replace=False)
X_labeled = X_pool[initial_indices]
```

2. **Cluster-based**: Sample from each cluster

```
kmeans = KMeans(n_clusters=10)
kmeans.fit(X_pool)
# Select one from each cluster
```

3. **Representative Sampling**: Use diversity methods

Active Learning Libraries

1. modAL

```
from modAL.models import ActiveLearner
from sklearn.ensemble import RandomForestClassifier

learner = ActiveLearner(
    estimator=RandomForestClassifier(),
    query_strategy=uncertainty_sampling,
    X_training=X_initial,
    y_training=y_initial
)

# Query 10 samples
query_idx, query_instance = learner.query(X_pool, n_instances=10)

# Teach with labels
learner.teach(X_pool[query_idx], y_pool[query_idx])
```

Complete Active Learning Example

```
from sklearn.datasets import make_classification
from sklearn.linear_model import LogisticRegression
import numpy as np

# Generate dataset
X, y = make_classification(n_samples=1000, n_features=20, n_classes=2)

# Split into initial labeled set and pool
n_initial = 20
initial_idx = np.random.choice(len(X), size=n_initial, replace=False)
X_labeled = X[initial_idx]
y_labeled = y[initial_idx]

pool_idx = np.setdiff1d(np.arange(len(X)), initial_idx)
X_pool = X[pool_idx]
y_pool = y[pool_idx]

# Active learning loop
model = LogisticRegression()
accuracies = []

for iteration in range(20):  # 20 iterations
    # Train model
    model.fit(X_labeled, y_labeled)

    # Evaluate
    score = model.score(X_test, y_test)
    accuracies.append(score)
    print(f"Iteration {iteration}: Accuracy = {score:.3f}")

    # Query most uncertain samples
    query_idx = uncertainty_sampling(model, X_pool, n_samples=10)

    # Simulate oracle labeling
    X_labeled = np.vstack([X_labeled, X_pool[query_idx]])
    y_labeled = np.hstack([y_labeled, y_pool[query_idx]])

    # Remove from pool
    X_pool = np.delete(X_pool, query_idx, axis=0)
    y_pool = np.delete(y_pool, query_idx, axis=0)
```

Simulating Oracles

For experiments, we need to simulate human labeling

Using existing labels:

```
def oracle(X_query, y_true, query_indices):
    # Return true labels for queried examples
    return y_true[query_indices]
```

With noise:

```
def noisy_oracle(y_true, query_indices, error_rate=0.1):
    labels = y_true[query_indices].copy()
    # Flip some labels randomly
    n_errors = int(len(labels) * error_rate)
    error_idx = np.random.choice(len(labels), size=n_errors, replace=False)
    labels[error_idx] = 1 - labels[error_idx]  # Flip binary labels
    return labels
```

Measuring Active Learning Performance

Learning Curve: Accuracy vs. number of labeled samples

```
import matplotlib.pyplot as plt

def plot_learning_curve(active_accuracies, random_accuracies, n_queries):
    plt.figure(figsize=(10, 6))

    x = np.arange(len(active_accuracies)) * n_queries

    plt.plot(x, active_accuracies, 'o-', label='Active Learning')
    plt.plot(x, random_accuracies, 's-', label='Random Sampling')

    plt.xlabel('Number of Labels')
    plt.ylabel('Accuracy')
    plt.title('Active Learning vs Random Sampling')
    plt.legend()
    plt.grid(True)
    plt.show()
```

Stopping Criteria

When to stop active learning?

1. **Budget exhausted**: Used all labeling budget
2. **Performance plateau**: Accuracy not improving
3. **Uncertainty threshold**: All examples have low uncertainty
4. **Time limit**: Deadline reached

Automatic stopping:

```
def should_stop(accuracies, window=3, threshold=0.01):
    if len(accuracies) < window:
        return False

    recent = accuracies[-window:]
    improvement = max(recent) - min(recent)
```

Active Learning for Deep Learning

Challenges:

- Deep models need more data
- Training is expensive
- Uncertainty estimation harder

Strategies:

1. **MC Dropout**: Use dropout at inference for uncertainty

```
# Enable dropout at test time
model.train()
predictions = [model(x) for _ in range(30)]
uncertainty = np.std(predictions, axis=0)
```

2. **Ensemble**: Train multiple models

Batch Mode Active Learning

Problem: Querying one example at a time is inefficient for deep learning

Solution: Query batches of examples

Challenge: Selected examples might be similar

Approaches:

1. **Top-k uncertain**: Simple, but may select similar examples
2. **Diverse batch**: Ensure batch covers feature space
3. **BatchBALD**: Maximize information about model parameters

```
def batch_uncertainty_sampling(model, X_unlabeled, batch_size=100):
    probs = model.predict_proba(X_unlabeled)
    uncertainties = 1 - np.max(probs, axis=1)

    # Select top-k
```

Active Learning with Label Studio

Label Studio: Open-source annotation tool with active learning

Features:

- Visual interface for labeling
- Built-in active learning
- Custom ML backends
- Export to various formats

Workflow:

1. Upload unlabeled data to Label Studio
2. Connect ML model
3. Model suggests next samples to label

Cost-Effectiveness Analysis

Compare labeling costs:

```
def cost_analysis(active_results, random_results, cost_per_label=1.0):
    target_accuracy = 0.90

    # Find labels needed for target accuracy
    active_labels = np.argmax(active_results >= target_accuracy) * 10
    random_labels = np.argmax(random_results >= target_accuracy) * 10

    active_cost = active_labels * cost_per_label
    random_cost = random_labels * cost_per_label

    savings = random_cost - active_cost
    savings_pct = (savings / random_cost) * 100

    print(f"Target Accuracy: {target_accuracy}")
    print(f"Active Learning: {active_labels} labels (${active_cost})")
    print(f"Random Sampling: {random_labels} labels (${random_cost})")
    print(f"Savings: ${savings} ({savings_pct:.1f}%)")
```

Domain Adaptation with Active Learning

Scenario: Model trained on domain A, deploying to domain B

Problem: Distribution shift causes poor performance

Solution: Use active learning to select examples from domain B

```
# Train initial model on source domain
model.fit(X_source, y_source)

# Active learning on target domain
X_pool = X_target  # Unlabeled target domain data

for iteration in range(n_iterations):
    # Query uncertain examples from target domain
    query_idx = uncertainty_sampling(model, X_pool, n_samples=batch_size)

    # Label (oracle)
    y_new = oracle(X_pool[query_idx])
```

Active Learning for Imbalanced Data

Problem: Rare classes get few queries with standard uncertainty sampling

Solution: Class-balanced active learning

```
def class_balanced_uncertainty_sampling(model, X_unlabeled, n_samples=10):
    probs = model.predict_proba(X_unlabeled)
    predicted_classes = np.argmax(probs, axis=1)
    uncertainties = 1 - np.max(probs, axis=1)

    selected = []
    samples_per_class = n_samples // len(np.unique(predicted_classes))

    for cls in np.unique(predicted_classes):
        cls_mask = predicted_classes == cls
        cls_uncertainties = uncertainties[cls_mask]
        cls_indices = np.where(cls_mask)[0]

        # Select most uncertain from this class
        top_k = min(samples_per_class, len(cls_indices))
```

Common Pitfalls

1. Not evaluating on separate test set

- Always use held-out test data
- Don't evaluate on the pool

2. Biased initial sample

- Start with diverse/representative sample
- Not just easiest examples

3. Ignoring computational cost

- Querying and retraining takes time
- Budget for compute, not just labels

4. Over-querying similar examples

Active Learning Best Practices

1. **Start small**: Begin with 5-10 examples per class
2. **Batch wisely**: Query 10-100 examples at once (depends on budget)
3. **Validate strategy**: Compare to random baseline
4. **Monitor convergence**: Track learning curves
5. **Consider human factors**:
    - Annotation fatigue
    - Label quality over time
    - Break large batches into sessions
6. **Save everything**: Log all queries and labels for analysis

Tools and Libraries

Active Learning:

- **modAL**: Python active learning framework
- **alipy**: Comprehensive active learning toolkit
- **libact**: C++ based, Python bindings

Annotation:

- **Label Studio**: Web-based with active learning
- **Prodigy**: Commercial, scriptable
- **CVAT**: Computer vision annotation
- **Labelbox**: Enterprise solution

Experiment tracking:

Real-World Case Studies

1. Medical Imaging (Chest X-rays)

- Random: 5,000 labels for 85% accuracy
- Active: 1,500 labels for 85% accuracy
- Savings: 70% reduction in radiologist time

2. Legal Document Review

- Random: 10,000 documents reviewed
- Active: 3,000 documents for same recall
- Savings: $140,000 in lawyer fees

3. Manufacturing Defect Detection

- Random: 1% defect rate, need 10,000 labels

Active Learning vs Other Approaches

Active Learning vs Semi-Supervised Learning:

- Active: Choose what to label
- Semi-supervised: Use unlabeled data directly

Active Learning vs Transfer Learning:

- Active: Label task-specific data intelligently
- Transfer: Use pretrained models

Active Learning vs Few-Shot Learning:

- Active: Iteratively grow labeled set
- Few-shot: Learn from very few examples (5-10)

Can combine! Transfer learning + active learning is powerful

Research Directions

Current trends:

1. **Deep active learning**: Better uncertainty for neural nets
2. **Active learning + RL**: Learn query strategy with RL
3. **Human-in-the-loop**: Better human-AI interaction
4. **Active learning at scale**: Billion-sample pools
5. **Weak supervision**: Combine with programmatic labeling

Open problems:

- Theoretical guarantees
- Better uncertainty estimation
- Handling label noise

Implementing Your First Active Learning System

Step-by-step:

1. **Load data**: Split into initial labeled set and pool
2. **Train initial model**: Use random sample
3. **Active learning loop**:
    - Predict on pool
    - Calculate uncertainty
    - Select top-k
    - Get labels (oracle or human)
    - Add to training set
    - Retrain model
4. **Evaluate**: Compare to random baseline

Practical Tips for Your Project

1. **Baseline is crucial**: Always compare to random sampling
2. **Start with toy dataset**: Test strategy on iris/digits
3. **Use existing labels**: Simulate oracle with held-out labels
4. **Track everything**:
    - Which samples were queried
    - Model performance at each iteration
    - Time spent
5. **Visualize uncertainty**: Plot samples by uncertainty to understand strategy
6. **Try multiple strategies**: Uncertainty, QBC, diversity

What We've Learned

Core Concepts:

- Active learning reduces labeling costs by 50-80%
- Query strategies: Uncertainty, QBC, diversity
- Oracle simulation for experiments
- Learning curves measure performance

Practical Skills:

- Implementing uncertainty sampling
- Building active learning loop
- Evaluating with learning curves
- Using libraries like modAL

Resources

Papers:

- "Active Learning Literature Survey" by Settles (2009)
- "Deep Active Learning" surveys
- "A Survey of Deep Active Learning" (2020)

Libraries:

- modAL: https://modal-python.readthedocs.io/
- Label Studio: https://labelstud.io/
- alipy: https://github.com/NUAA-AL/alipy

Datasets:

- MNIST, CIFAR-10 for experiments

Bayesian Active Learning

Bayesian Perspective: Uncertainty about model parameters θ

Posterior after seeing data $\mathcal{D}$:

$$P(\theta|\mathcal{D}) = \frac{P(\mathcal{D}|\theta)P(\theta)}{P(\mathcal{D})}$$

Predictive distribution:

$$P(y|x, \mathcal{D}) = \int P(y|x, \theta)P(\theta|\mathcal{D})d\theta$$

Uncertainty comes from:

1. **Aleatoric**: Inherent data noise
2. **Epistemic**: Model uncertainty (reducible with more data)

BALD: Bayesian Active Learning by Disagreement

Goal: Maximize information gain about model parameters

Information Gain:

$$I(y; \theta | x, \mathcal{D}) = H(y|x, \mathcal{D}) - \mathbb{E}_{P(\theta|\mathcal{D})}[H(y|x, \theta)]$$

Components:

- $H(y|x, \mathcal{D})$: Entropy of predictive distribution (uncertainty)
- $\mathbb{E}[H(y|x, \theta)]$: Expected conditional entropy (noise)

Difference = epistemic uncertainty (what active learning should target)

Implementation (with MC Dropout):

```
def bald_acquisition(model, x, n_samples=30):
    """BALD acquisition function using MC Dropout."""
    # Enable dropout at inference
    model.train()
```

BatchBALD: BALD for Batches

Problem: BALD is for single queries, but we want batches

Naive approach: Select top-k BALD scores

Issue: May select redundant examples

BatchBALD: Maximize joint information gain

Joint Mutual Information:

$$I(\{y_1, \ldots, y_b\}; \theta | \{x_1, \ldots, x_b\}, \mathcal{D})$$

Greedy approximation:

1. Select x_1 with highest BALD score
2. Select x_2 with highest conditional information gain given x_1
3. Repeat for batch size b

Expected Error Reduction: Detailed Theory

Goal: Select examples that minimize expected future error

Expected Error after labeling (x, y):

$$\mathbb{E}_{P(y|x)}[L(\mathcal{D} \cup \{(x, y)\})]$$

where $L(\mathcal{D})$ is loss on validation set given training set $\mathcal{D}$

Algorithm:

1. For each unlabeled x_i
2. For each possible label y:
    - Compute $P(y|x_i)$
    - Simulate adding (x_i, y) to training set
    - Retrain model → compute validation loss

Expected Error Reduction: Implementation

```python
def expected_error_reduction(model, X_unlabeled, X_val, y_val, n_samples=5):
    """Approximate expected error reduction."""
    expected_errors = []

    for x in X_unlabeled:
        # Get prediction probabilities
        probs = model.predict_proba([x])[0]

        # For each possible label
        expected_error = 0
        for y, prob in enumerate(probs):
            # Simulate adding (x, y) to training set
            # (In practice, use gradient approximation instead of retraining)

            # Approximate: train model with new example
            model_copy = clone(model)
            X_train_new = np.vstack([X_labeled, [x]])
            y_train_new = np.hstack([y_labeled, [y]])
            model_copy.fit(X_train_new, y_train_new)

            # Compute validation error
            val_error = 1 - model_copy.score(X_val, y_val)

            # Weight by probability
            expected_error += prob * val_error

        expected_errors.append(expected_error)

    # Select sample with minimum expected error
    return np.argmin(expected_errors)
```

Version Space and Active Learning

Version Space: Set of all hypotheses consistent with training data

$$VS_{\mathcal{D}} = \{h \in \mathcal{H} : h(x) = y \text{ for all } (x, y) \in \mathcal{D}\}$$

Query-by-Committee samples from version space:

- Each committee member represents a hypothesis in VS
- Disagreement → large version space → more uncertainty

Optimal query (theoretically):

- Cuts version space in half
- Maximizes expected reduction in version space size

Generalized Binary Search:

$$x^* = \arg\max_x \min_y |VS_{\mathcal{D} \cup \{(x,y)\}}|$$

PAC Learning Bounds for Active Learning

PAC (Probably Approximately Correct): With probability $1 - \delta$, achieve error $\leq \epsilon$

Passive learning label complexity:

$$m_{passive} = O\left(\frac{d \log(1/\epsilon)}{\epsilon}\right)$$

where d = VC dimension

Active learning label complexity (linear separators):

$$m_{active} = O\left(d \log^2\left(\frac{1}{\epsilon}\right)\right)$$

Improvement: Exponential in ϵ for some hypothesis classes!

Disagreement coefficient θ:

Stream-Based Active Learning

Pool-based: Have entire unlabeled pool, select best examples

Stream-based: Examples arrive sequentially, decide to label or skip

Decision function:

$$\text{label}(x) = \begin{cases} \text{true} & \text{if } U(x) > \tau \\ \text{false} & \text{otherwise} \end{cases}$$

where τ is threshold

Adaptive threshold:

```
class StreamActiveLearner:
    def __init__(self, model, budget):
        self.model = model
        self.budget = budget
        self.labeled_count = 0
        self.threshold = 0.5  # Initial threshold

    def process_stream(self, x):
        """Decide whether to label incoming example."""
```

Membership Query Synthesis

Standard active learning: Select from unlabeled pool

Membership query: Generate/synthesize queries

Example (linear classifier):

- Decision boundary is $w^T x = 0$
- Generate query on decision boundary
- Most informative for refining boundary

Synthetic query generation:

```
def generate_boundary_query(model, X_pool):
    """Generate query on decision boundary."""
    # Find two examples from different classes
    probs = model.predict_proba(X_pool)
    preds = np.argmax(probs, axis=1)
```

Multi-Label Active Learning

Multi-label: Each example can have multiple labels

Example: Image tagging - "beach", "sunset", "people"

Uncertainty measures:

1. Min-max uncertainty:

$$U(x) = \max_l P(l|x) - \min_l P(l|x)$$

2. Avg uncertainty across labels:

$$U(x) = \frac{1}{L} \sum_{l=1}^{L} H(P(y_l|x))$$

3. Label cardinality uncertainty:

Active Feature Acquisition

Scenario: Features are costly to obtain (medical tests, sensors)

Goal: Decide which features AND which examples to acquire

Decision:

1. **Example selection**: Which instance to label?
2. **Feature selection**: Which features to measure for that instance?

Value of information:

$$VOI(f_i, x) = I(y; f_i | x, \mathcal{D})$$

Joint optimization:

```
def active_feature_acquisition(model, X_partial, feature_costs):
    """Select which feature to acquire for which sample."""
    best_value = -np.inf
    best_sample = None
```

Active Learning with Label Noise

Problem: Oracle labels can be noisy (human errors)

Strategies:

1. **Repeated labeling**:

- Label uncertain examples multiple times
- Use majority vote or probabilistic aggregation

2. **Confidence-weighted sampling**:

```
def noise_robust_sampling(model, X_unlabeled, n_samples=10):
    """Uncertainty sampling robust to label noise."""
    probs = model.predict_proba(X_unlabeled)
    uncertainties = 1 - np.max(probs, axis=1)

    # Downweight very hard examples (likely noise)
    # Weight by difficulty
```

Adversarial Active Learning

Goal: Robustness to adversarial examples

Adversarial uncertainty:

```
def adversarial_active_learning(model, X_unlabeled, epsilon=0.1):
    """Select examples near adversarial decision boundary."""
    uncertainties = []

    for x in X_unlabeled:
        # Compute gradient
        x_tensor = torch.tensor(x, requires_grad=True)
        output = model(x_tensor)
        loss = -torch.max(output)  # Negative to find worst case
        loss.backward()

        # Generate adversarial perturbation
        perturbation = epsilon * torch.sign(x_tensor.grad)
        x_adv = x_tensor + perturbation

        # Measure uncertainty on adversarial example
        adv_probs = model(x_adv).detach().numpy()
        adv_uncertainty = 1 - np.max(adv_probs)
```

Budget-Constrained Active Learning

Constraint: Total labeling budget B

Variable costs: Different samples have different labeling costs

Optimization:

$$\max_{\mathcal{S}} \text{Information}(\mathcal{S}) \quad \text{s.t.} \quad \sum_{x \in \mathcal{S}} c(x) \leq B$$

Cost-aware acquisition:

```python
def cost_aware_active_learning(model, X_unlabeled, costs, budget):
    """Active learning with variable annotation costs."""
    selected = []
    remaining_budget = budget

    while remaining_budget > 0:
        # Get uncertainties
        probs = model.predict_proba(X_unlabeled)
        uncertainties = 1 - np.max(probs, axis=1)

        # Compute value = uncertainty / cost
        values = uncertainties / costs
```

Regret Bounds for Active Learning

Regret: Difference between optimal and actual performance

Cumulative regret after T queries:

$$R(T) = \sum_{t=1}^{T} L(h_t) - L(h^*)$$

where:

- $L(h_t)$: Loss of model at iteration t
- $L(h^*)$: Loss of optimal model

Goal: Minimize regret

Upper bound (for some algorithms):

$$R(T) = O(\sqrt{T \log T})$$

Exploration-Exploitation Tradeoff

Exploration: Query uncertain examples (learn model)

Exploitation: Query high-value examples (improve specific regions)

Thompson Sampling for active learning:

```
class ThompsonSamplingAL:
    def __init__(self, model, n_models=10):
        self.models = [clone(model) for _ in range(n_models)]

    def query(self, X_unlabeled, X_labeled, y_labeled):
        """Thompson sampling for active learning."""
        # Train multiple models on bootstrap samples
        for model in self.models:
            # Bootstrap sample
            idx = np.random.choice(len(X_labeled), size=len(X_labeled), replace=True)
            model.fit(X_labeled[idx], y_labeled[idx])

        # Sample one model
        sampled_model = np.random.choice(self.models)
```

Contextual Bandits and Active Learning

Connection: Active learning as contextual bandit problem

Contextual bandit:

- Context: Unlabeled example x
- Actions: Label or skip
- Reward: Information gain

Upper Confidence Bound (UCB):

$$\text{Score}(x) = \bar{U}(x) + \sqrt{\frac{2 \log t}{n(x)}}$$

where:

- $\bar{U}(x)$: Average uncertainty for examples similar to x

Active Learning for Structured Prediction

Structured output: Sequences, trees, graphs (NER, parsing, segmentation)

Challenge: Output space is exponential

Uncertainty measures:

1. **Sequence entropy**:

$$H(y|x) = -\sum_{y \in \mathcal{Y}} P(y|x) \log P(y|x)$$

2. **Token-level uncertainty** (for sequences):

$$U(x) = \frac{1}{|x|} \sum_{t=1}^{|x|} H(y_t|x)$$

3. **N-best list diversity**:

Active Learning for Ranking

Goal: Learn ranking function with minimal labeled pairs

Pairwise comparison: "Is A better than B?"

Uncertainty for pairs:

$$U(x_i, x_j) = |P(x_i \succ x_j) - 0.5|$$

Pairs close to 0.5 are most uncertain

Query selection:

```
def active_learning_for_ranking(model, items):
    """Active learning for learning-to-rank."""
    uncertainties = []

    # Consider all pairs
    for i, x_i in enumerate(items):
        for j, x_j in enumerate(items):
```

Active Learning for Clustering

Unsupervised active learning: Query pairwise constraints

Types of queries:

1. **Must-link**: Do x_i and x_j belong to same cluster?
2. **Cannot-link**: Do x_i and x_j belong to different clusters?

Constrained K-means:

```
def active_learning_clustering(X, n_clusters, budget):
    """Active learning for clustering."""
    must_link = []
    cannot_link = []

    for _ in range(budget):
        # Initial clustering
        kmeans = KMeans(n_clusters=n_clusters)
        clusters = kmeans.fit_predict(X)

        # Find most uncertain pair
        # (close in feature space but in different clusters)
        uncertainties = []
        for i in range(len(X)):
            for j in range(i+1, len(X)):
                dist = np.linalg.norm(X[i] - X[j])
                same_cluster = clusters[i] == clusters[j]

                # Uncertainty = close but different cluster OR far but same cluster
                if same_cluster:
```

Lifelong Active Learning

Scenario: Multiple related tasks over time

Goal: Transfer knowledge across tasks to reduce labeling

Approach:

1. Learn task T_1 with active learning
2. For task T_2, use knowledge from T_1 to initialize
3. Active learning on T_2 with transfer

```
class LifelongActiveLearner:
    def __init__(self, base_model):
        self.tasks = []
        self.models = []

    def learn_task(self, X_pool, y_pool, budget):
        """Learn new task with active learning."""
        # Transfer from previous tasks
        if self.models:
            # Initialize with previous model
            model = clone(self.models[-1])
        else:
            # First task
            model = clone(self.base_model)
```

Online Active Learning

Setting: Examples arrive in stream, must decide immediately

No look-ahead: Can't compare to future examples

Challenge: Balance immediate labeling vs waiting for better example

Threshold-based online active learning:

```
class OnlineActiveLearner:
    def __init__(self, model, budget, stream_size):
        self.model = model
        self.budget = budget
        self.stream_size = stream_size
        self.labeled_count = 0
        self.seen_uncertainties = []

    def process_example(self, x, y_true):
        """Process one example from stream."""
        # Predict uncertainty
        if hasattr(self.model, 'predict_proba'):
            probs = self.model.predict_proba([x])[0]
            uncertainty = 1 - np.max(probs)
        else:
            # Random if model not trained yet
            uncertainty = 0.5

        self.seen_uncertainties.append(uncertainty)

        # Adaptive threshold based on budget
```

Distributed Active Learning

Scenario: Multiple agents/annotators working in parallel

Challenges:

1. Coordination: Avoid querying same examples
2. Communication: Share model updates
3. Synchronization: Merge labels and retrain

Distributed uncertainty sampling:

```
class DistributedActiveLearner:
    def __init__(self, model, n_agents):
        self.global_model = model
        self.n_agents = n_agents
        self.agent_models = [clone(model) for _ in range(n_agents)]

    def distributed_query(self, X_pool, n_samples_per_agent):
        """Query examples for each agent."""
        all_queries = []

        for agent_id in range(self.n_agents):
            # Each agent uses global model
            probs = self.global_model.predict_proba(X_pool)
            uncertainties = 1 - np.max(probs, axis=1)
```

Privacy-Preserving Active Learning

Goal: Active learning without exposing sensitive data

Federated active learning:

- Data stays on client devices
- Only model updates shared

Differential privacy:

- Add noise to queries and labels
- Preserve privacy while learning

```
class PrivacyPreservingActiveLearner:
    def __init__(self, model, epsilon=1.0):
        self.model = model
        self.epsilon = epsilon  # Privacy budget

    def private_uncertainty(self, X_unlabeled):
        """Compute uncertainty with differential privacy"""
```

Fairness in Active Learning

Problem: Active learning may bias towards majority groups

Fair active learning: Ensure diverse coverage across demographic groups

```
def fair_active_learning(model, X_unlabeled, groups, n_samples=10):
    """Active learning with fairness constraints."""
    unique_groups = np.unique(groups)
    samples_per_group = n_samples // len(unique_groups)

    selected = []

    for group in unique_groups:
        # Get samples from this group
        group_mask = groups == group
        X_group = X_unlabeled[group_mask]
        group_idx = np.where(group_mask)[0]

        # Uncertainty sampling within group
        probs = model.predict_proba(X_group)
        uncertainties = 1 - np.max(probs, axis=1)
```

Advanced Active Learning Summary

Theoretical Foundations:

- Bayesian active learning (BALD, BatchBALD)
- PAC learning bounds
- Version space reduction
- Regret bounds

Advanced Strategies:

- Expected error reduction
- Membership query synthesis
- Exploration-exploitation (Thompson sampling, UCB)

Specialized Settings:

Questions?

Next: Data Augmentation

Lab: Build active learning system from scratch