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tags :

- Machine Learning
- Hands on ML - book

Chapter 4 - Hands on

- This chapter dives into how machine learning models work under the hood. It covers:
  - **Linear Regression** using closed-form solutions and **Gradient Descent** (plus its variants).
  - **Polynomial Regression**, overfitting, and how to prevent it with **learning curves** and **regularization**.
  - **Logistic** and **Softmax Regression** for classification tasks.

Linear Regression

- What is Linear Regression?
  - It's a model that predicts an output by computing a **weighted sum of input features**, plus a **bias** (intercept).
  - The general form is:
    $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$
  - In vector form:
    $\hat{y} = \theta^T \cdot x$
  - (where θ is the vector of parameters, and x is the vector of input features including a 1 for the bias term)
- How Do We Train It?
  - We adjust θ (the model's parameters) to best fit the training data.
  - To measure how well it fits, we use **Mean Squared Error (MSE)** as the cost/loss function:
  - This helps us find the values of θ that minimize prediction errors.
- Training loss (like MSE) is optimized during training.
- Evaluation metrics (like precision/recall) may differ from training loss, especially for classifiers.
- Good loss functions are **easy to optimize** and **correlate with real-world goals**.

The Normal Equation

- What is the **Normal Equation**?
  - It's a **direct formula** to compute the best parameters **θ** that minimize the MSE (no iteration needed):
- How It Works:
  1. Generate training data with some noise:
  2. Add a column of 1s to `X` (to handle the bias term).
  3. Use NumPy to compute **θ** directly using matrix operations.
  4. Predictions are made by multiplying new input data by the computed **θ**.
- Example Results:
  - The true parameters were 4 and 3.
  - The model estimated them as **4.215** and **2.770** — close, but slightly off due to noise.
- Using Scikit-Learn:
  - You can use `LinearRegression()` from scikit-learn to do the same thing with `.fit()` and `.predict()`.
  - It separates the **intercept_** (bias) and **coef_** (feature weights).
- **Pseudoinverse Alternative:**
  - Instead of using the Normal Equation, you can use the **pseudoinverse**:

    - is the of X. Computed using `np.linalg.pinv(X)`
    - More stable and handles edge cases where $X^T X$ is not invertible (e.g., redundant features or too few data points).
- **Normal Equation** is a fast, direct way to compute parameters for linear regression.
- **Pseudoinverse** is more robust and always works, even when the Normal Equation fails.
- Libraries like **scikit-learn** and **NumPy** make it easy to use both.

Computational Complexity

- Normal Equation & SVD Complexity:
  - **Normal Equation** has a complexity of about **O() to O()** → gets **slow with many features**.
  - **SVD** (used by Scikit-Learn) is about **O(n²)** → still slow when **n (features)** is very large.
  - **Both handle large datasets (many rows, m) well**, since they are **linear in m**: **O(m)**.
- Prediction Time:
  - Once the model is trained, making predictions is **very fast**.
  - Time grows **linearly** with the number of instances and features.

Gradient Descent

- What is Gradient Descent?

    - An **optimization algorithm** that finds the best model parameters (like θ) by minimizing a **cost function** (e.g., MSE).
    - It does this by **iteratively moving in the direction of the steepest slope** (i.e., negative gradient).
- How It Works:
    1. **Start** with random parameter values (random initialization).
    2. Repeatedly **adjust parameters** to reduce the cost.
    3. **Stop when** the gradient becomes zero → minimum reached.
- Learning Rate (Step Size):
    - **Too small** → slow convergence (takes many steps).
    - **Too large** → may overshoot or diverge (never settles).
    - Must choose a **balanced learning rate**!
- hallenges:
    - Some cost functions can have **plateaus, local minima**, or **complex shapes**.
    - BUT for **linear regression**, the MSE cost function is:
        - ✅ **Convex** (no local minima)
        - ✅ **Smooth** (no sharp changes)
        - ➡️ So, gradient descent is **guaranteed** to find the global minimum eventually.
- Feature Scaling:
    - If features have **different scales**, gradient descent:
        - Takes weird zigzag paths,
        - Converges **very slowly**.
    - Use tools like `StandardScaler` to **normalize** feature scales.

Batch Gradient Descent

- **What is Batch Gradient Descent?**
    - Batch Gradient Descent is an optimization algorithm used to **minimize the cost function** (like MSE in linear regression) by adjusting model parameters .
- **Key Concepts**
    1. **Cost Function (MSE)**
       Measures how bad the model's predictions are:
    2. **Gradient (Slope Vector)**
       Tells you how to tweak to reduce the error. It's the vector of **partial derivatives** of the cost function with respect to each parameter .
        - manual for each paramete :
        - vectorized for all parameters :

3. Gradient Descent Update Rule
   Use the gradient to update θ by taking a step **opposite the slope**:
   - = learning rate (step size)
4. **Code :-**

```
eta = 0.1            # learning rate
n_epochs = 1000      # number of passes over the dataset
m = len(X_b)         # number of samples

theta = np.random.randn(2, 1)  # random initialization

for epoch in range(n_epochs):
    gradients = 2 / m * X_b.T @ (X_b @ theta - y)
    theta = theta - eta * gradients
```

5. Learning Rate Matters
   - **Too small** → very slow convergence
   - **Just right** → fast and stable
   - **Too large** → divergence (jumps around, doesn't settle)
6. **When to Stop?**
   - Set a max number of epochs, **or**
   - Stop early when the gradient becomes very small (i.e., close to minimum)
7. **Convergence**
   - Gradient descent will converge for convex functions like MSE
   - The convergence speed depends on the **learning rate** and **tolerance**

Stochastic Gradient Descent

- **What is SGD?**
  - Unlike **Batch Gradient Descent** (which uses the whole dataset per step), **SGD** uses **only one random data point per update**.
  - This makes each step much **faster** and allows training on very **large datasets**.
- **Pros and Cons**
  - pros
    - Faster updates
    - Can escape local minima
    - Scalable to huge datasets
  - Cons
    - More noisy (bouncy) path to minimum
    - Doesn’t settle exactly at the minimum
    - May require careful tuning of learning rate

- **Epochs and Iterations**
  - One **epoch** = one full pass through the dataset.
  - Each **epoch** consists of `m` **updates** (one per training example).
  - If random sampling is used, some examples might be picked multiple times or not at all in one epoch.
- **Learning Rate Schedule**
  - To reduce noise and allow convergence, **learning rate should shrink over time**.
  - This is done using a **learning schedule**, e.g.:

    ```
    def learning_schedule(t):
        return t0 / (t + t1)
    ```

  - Starts with larger steps (fast progress), then gets smaller (finer tuning).
- **Important Considerations**
  - Data must be **IID (independent and identically distributed)** — shuffle it!
  - If data is ordered (e.g., by label), SGD can behave badly.
- **SGD in Code**
  - ```
    for epoch in range(n_epochs):
        for iteration in range(m):  # m training instances
            random_index = np.random.randint(m)
            xi = X_b[random_index : random_index + 1]
            yi = y[random_index : random_index + 1]
            gradients = 2 * xi.T @ (xi @ theta - yi)
            eta = learning_schedule(epoch * m + iteration) # t which is the
    i/p of learning_schedule
            theta = theta - eta * gradients
    ```

- **Scikit-Learn's SGDRegressor**
  - ```
    from sklearn.linear_model import SGDRegressor
    sgd_reg = SGDRegressor(
        max_iter=1000, tol=1e-5, eta0=0.01, penalty=None,
        n_iter_no_change=100, random_state=42
    )
    sgd_reg.fit(X, y.ravel())
    ```

Mini-Batch Gradient Descent

- Mini-batch Gradient Descent (MBGD) is a hybrid between:
  - **Batch GD**: Uses the whole dataset per step (slow but stable).
  - **Stochastic GD (SGD)**: Uses 1 sample per step (fast but noisy).
- **MBGD** uses **small random batches** of data (e.g. 32 or 64 samples).

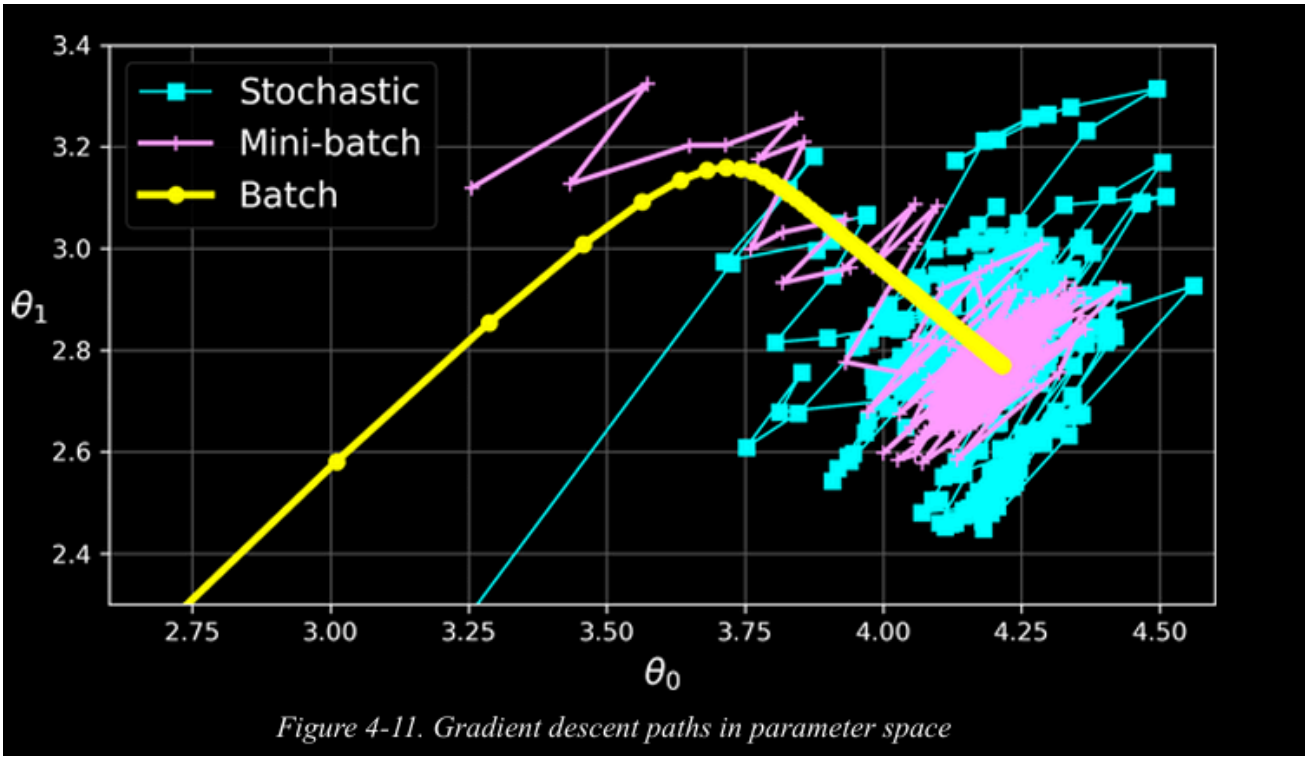
- **Advantages**
  - Faster than Batch GD.
  - Less noisy than SGD.
  - Can benefit from hardware acceleration (like GPUs).
  - Works well with **large datasets**.
- **Disadvantages**
  - Still bounces around the minimum (but less than SGD).
  - Might get stuck in local minima (especially for non-convex problems).
  - Needs a learning schedule (like SGD).
- 

Figure 4-11. Gradient descent paths in parameter space
  - **Batch GD** : smooth, direct to the minimum, stops there.
  - **Stochastic GD** : very noisy path, keeps bouncing.
  - **Mini-batch GD** : less noisy than SGD, ends near the minimum.

Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	n/a
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	`SGDRegressor`
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`

Polynomial Regression

- **Polynomial Regression Overview**
  - **Goal**: Fit **nonlinear data** using a **linear model**.
  - **How**: Add **powers of features** (e.g. etc.) as **new features**, then apply **linear regression**.
- **Example Process**:
  1. **Generate nonlinear data**:
     -
  2. **Use** `PolynomialFeatures` from `sklearn`:
     - ```
       from sklearn.preprocessing import PolynomialFeatures
       poly_features = PolynomialFeatures(degree=2, include_bias=False)
       X_poly = poly_features.fit_transform(X)
       ```
     - Turns into
  3. **Train Linear Regression** on transformed data:
     - ```
       from sklearn.linear_model import LinearRegression
       lin_reg = LinearRegression()
       lin_reg.fit(X_poly, y)
       ```
- **Model Output Example**:
  - The model learns:
  - Close to the original:
- **Key Points**:
  - **Polynomial regression ≠ nonlinear model** — it's still **linear in parameters**.
  - When multiple features are present, **interactions** (e.g.,) are added automatically.

- **Warning**: With high degree `d` and many features `n`, the number of features grows **combinatorially**:
- Increasing polynomial degree can **cause overfitting**.

Learning Curves

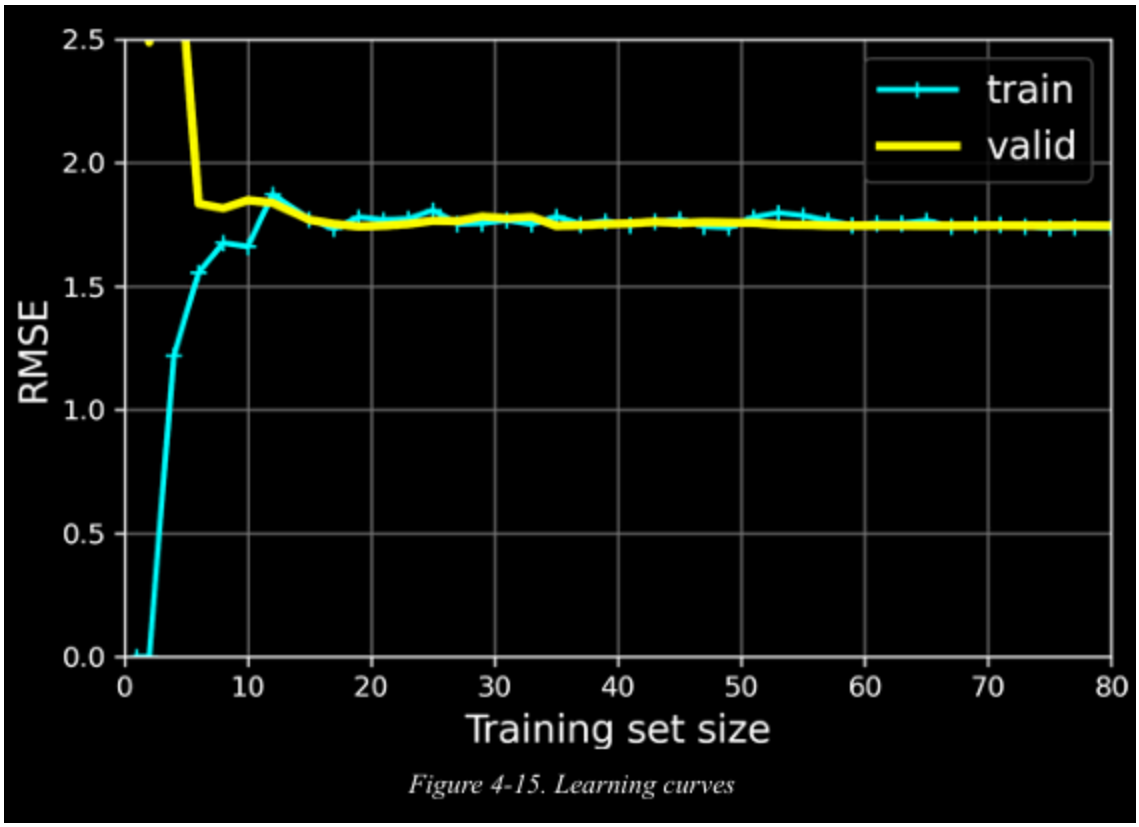
- What Are They?
  - **Plots of:** Training error and Validation error vs. Training set size.
  - Help diagnose:
    - **Underfitting** (high bias)
    - **Overfitting** (high variance)
- Key Observations
  - **Underfitting Example (Linear Model)**:
    

    Figure 4-15. Learning curves
    - **Training error**: Starts low (small data) then rises and plateaus
    - **Validation error**: Starts high, decreases, then plateaus near training error
    - → **Both errors high & close** = Model too simple (high bias)
  - **Overfitting Example (10th-degree Polynomial)**:

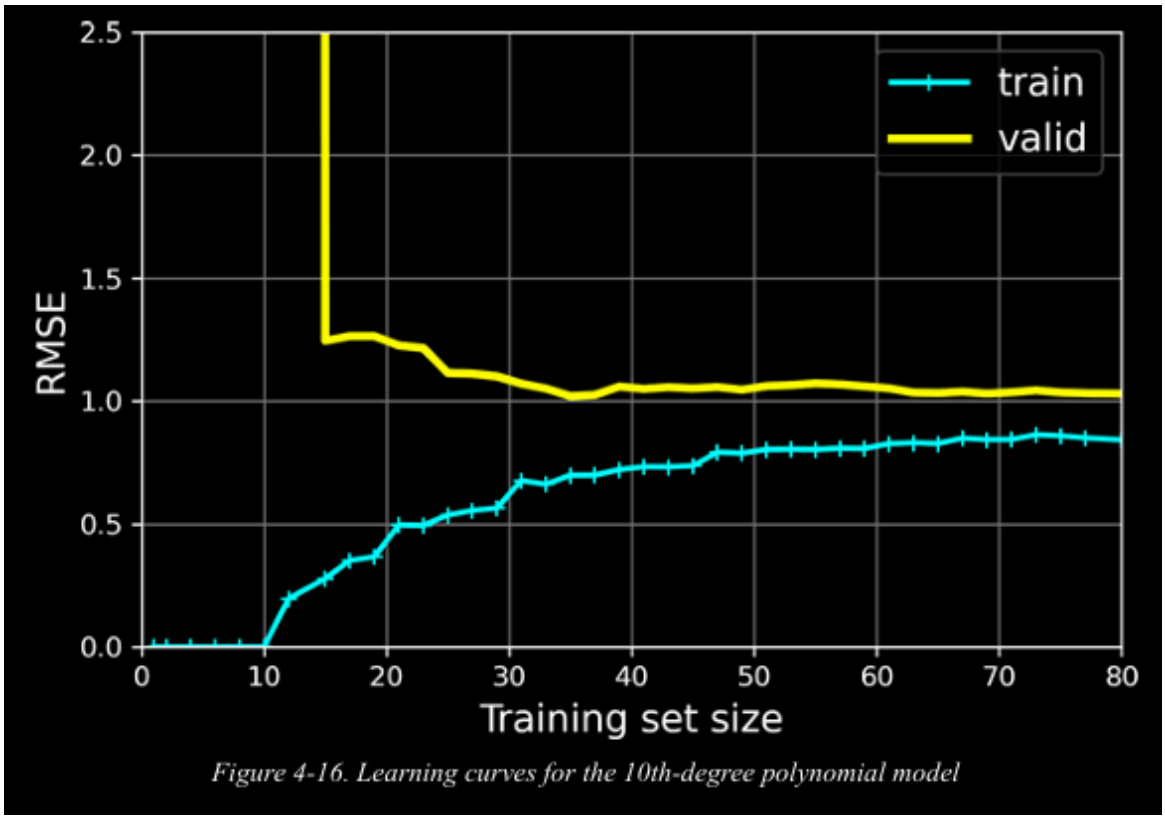


Figure 4-16. Learning curves for the 10th-degree polynomial model

- **Training error**: Very low
- **Validation error**: Higher and doesn't match training error
- → **Big gap between curves** = Model too complex (high variance)
- ✅ Can often fix with **more training data**

- **Tips:**
  - **Underfitting?** → Try a more complex model or better features
  - **Overfitting?** → Try regularization or add more data
  - **Irreducible error?** → Clean up your dataset

Regularized Linear Models

- **Regularization** helps reduce **overfitting** by limiting model complexity.
- For **polynomial models**, reduce the **degree**.
- For **linear models**, **constrain the weights** using:
  1. **Ridge Regression (L2)** – Shrinks all weights.
  2. **Lasso Regression (L1)** – Shrinks some weights to **zero** (feature selection).
  3. **Elastic Net** – Mix of L1 and L2 regularization.

Ridge Regression

- What Is Ridge Regression?
  - **Ridge Regression** (aka **Tikhonov regularization**) is **Linear Regression + L2 regularization**.

    - The goal: Fit the data **while keeping model weights small**, reducing overfitting.
- **Cost Function**
    -
    - Adds a **penalty** for large weights.
    - Bias term is **not** regularized.
    - controls regularization strength:
        - = 0→ plain Linear Regression.
        - Large → very flat model.
- **Important: Always Scale Your Features**
    - Use `StandardScaler` before applying Ridge. Regularization is sensitive to feature scales.
- **Intuition**
    - **High** → simple, flat predictions → **low variance**, **high bias**.
    - **Low** → **more flexible model** → **low bias**, **high variance**.
    - This helps manage the **bias-variance trade-off**.
- **How To Use Ridge in Scikit-Learn**
    1. Closed-form (exact solution):

```
from sklearn.linear_model import Ridge
ridge_reg = Ridge(alpha=0.1, solver="cholesky")
ridge_reg.fit(X, y)
ridge_reg.predict([[1.5]])
```

    2. Using Stochastic Gradient Descent (SGD):

```
from sklearn.linear_model import SGDRegressor
sgd_reg = SGDRegressor(penalty="l2", alpha=0.1/m, tol=None,
                       max_iter=1000, eta0=0.01, random_state=42)
sgd_reg.fit(X, y.ravel())  # y must be 1D
sgd_reg.predict([[1.5]])
```

- **Extra Tip: Automatic Tuning**
    - Use `RidgeCV` for **automatic α tuning** with cross-validation:

```
from sklearn.linear_model import RidgeCV
ridge_cv = RidgeCV(alphas=[0.01, 0.1, 1.0, 10.0])
ridge_cv.fit(X, y)
```

Lasso Regression

- **What is Lasso Regression?**
    - **Lasso** stands for **Least Absolute Shrinkage and Selection Operator**.

- It's a regularized version of **linear regression** that adds an **ℓ_1 (absolute value) penalty** to the cost function.

- Cost Function:

  - ℓ_1 norm = sum of absolute values of the weights (no squares like Ridge).
  - This encourages some weights to become exactly **zero → feature selection**!

- **Effect of Lasso:**
  - Can **zero out** unimportant features, making the model **sparse** and easier to interpret.
  - Increasing **α** increases regularization (more weights shrink to zero).
  - Decreasing **α** moves the solution toward plain linear regression (no regularization).
- **Gradient and Subgradient:**
  - Lasso's cost function is **not differentiable at θ = 0**.
  - Gradient descent uses a **subgradient** instead:
    - `sign(θ_i)` is used: returns -1, 0, or 1 based on the sign of each θ.
- You can also use `SGDRegressor(penalty="l1")` to perform lasso-style training with SGD.
- Scikit-Learn Example:

```
from sklearn.linear_model import Lasso

lasso_reg = Lasso(alpha=0.1)
lasso_reg.fit(X, y)
lasso_reg.predict([[1.5]])
# Output: array([1.53788174])
```

Elastic Net Regression

- **What is Elastic Net?**
  - **Elastic Net** combines both **Ridge (ℓ_2)** and **Lasso (ℓ_1)** penalties.
  - It's a **weighted average** of Ridge and Lasso regularization.
- **Cost Function:**
  - `r = 0`: behaves like **Ridge**
  - `r = 1`: behaves like **Lasso**
- **When to Use Elastic Net?**
  - Use **regularization** in general (avoid plain linear regression).
  - **Ridge** is a good default.
  - Use **Lasso/Elastic Net** if you believe:
    - Only a few features are important
    - You want **automatic feature selection**
  - Prefer **Elastic Net** over Lasso when:

    - You have **more features than samples**
    - Some features are **highly correlated**
- Scikit-Learn Example:

```
from sklearn.linear_model import ElasticNet

elastic_net = ElasticNet(alpha=0.1, l1_ratio=0.5)  # l1_ratio = r
elastic_net.fit(X, y)
elastic_net.predict([[1.5]])
# Output: array([1.54333232])
```

Early Stopping

- **What is Early Stopping?**
    - A **regularization technique** for iterative learning (like gradient descent).
    - You **stop training** when the **validation error stops improving**.
    - Helps **prevent overfitting** by not overtraining the model.
    - Called a "**beautiful free lunch**" by Geoffrey Hinton because it's simple yet powerful.
- **How It Works (Conceptually)**
    - During training:
        - Training error keeps going **down**.
        - Validation error goes **down**, then **up** (indicating overfitting).
    - **Early stopping** halts training **at the lowest validation error**, before overfitting begins.
- **Code**
    1. Data Prep

```
X_train, y_train, X_valid, y_valid = [...]  # split dataset

preprocessing = make_pipeline(
                    PolynomialFeatures(degree=90, include_bias=False),
                    StandardScaler())
X_train_prep = preprocessing.fit_transform(X_train)
X_valid_prep = preprocessing.transform(X_valid)
```

    2. Model Setup

```
sgd_reg = SGDRegressor(penalty=None, eta0=0.002, random_state=42)
```

        - Uses **Stochastic Gradient Descent** (SGD).
        - **No regularization** (`penalty=None`).
        - Small learning rate `eta0=0.002` .
    3. Training with Early Stopping

```python
from copy import deepcopy
n_epochs = 500
best_valid_rmse = float('inf')  # start with the worst possible error

for epoch in range(n_epochs):
    sgd_reg.partial_fit(X_train_prep, y_train)  # train one step
    y_valid_predict = sgd_reg.predict(X_valid_prep)
    val_error = mean_squared_error(y_valid, y_valid_predict,
squared=False)  # RMSE

    if val_error < best_valid_rmse:  # if new best
        best_valid_rmse = val_error
        best_model = deepcopy(sgd_reg)  # save current model
```

Logistic Regression

- A classification algorithm (despite its name).
- Predicts the **probability** an instance belongs to class **1** (positive class).
- If probability > 50%, it predicts **1**, else **0** (negative class).
- Used for **binary classification** problems (e.g., spam detection).

Estimating Probabilities

- Logistic regression computes:

- Output is a **probability** between 0 and 1.
- Prediction rule:
  - If ≥ 0.5, predict class **1**.
  - If < 0.5, predict class **0**.

Training and Cost Function

- Train the model so that:
  - High probabilities for **positive class (y = 1)**
  - Low probabilities for **negative class (y = 0)**
- Single Instance Cost
  -
- Total Cost (Log Loss)
  -
    - Called **log loss**, and it's **convex**, so Gradient Descent can find the **global minimum**.

- Gradient
  -
  - Same idea as linear regression: error × feature → average over all samples.
  - Used in **batch, stochastic**, or **mini-batch Gradient Descent** to update weights.

Decision Boundaries

- Dataset Used: Iris Dataset
  - 150 iris flowers, 3 species: **Setosa**, **Versicolor**, **Virginica**
  - Features: sepal/petal **length** and **width**
- **Goal:**
  - Classify **whether a flower is Iris Virginica** based on petal width.
- **Steps:**
  1. **Load data** using `load_iris()`
  2. **Use only petal width** as input feature
  3. Create binary labels:
     `y = True` if **Virginica**, `False` otherwise
  4. **Split data** → Train/Test
  5. **Train** logistic regression model with `fit()`
  6. **Predict probabilities** with `predict_proba()`
- **Decision Boundary:**
  - Model predicts **Virginica** if **probability ≥ 0.5**
  - This creates a **threshold (decision boundary)** at **~1.65 cm**
  - If **petal width > 1.65 cm** → **Virginica**, else not

Softmax Regression

- Softmax Regression is a generalization of logistic regression that works for multiple classes directly — no need to train separate binary classifiers.
- **How It Works (Prediction)**
  1. For an input , the model calculates a **score** for each class:
     ,Each class has its own weight vector
  2. It then applies the **softmax function** to convert these scores into **probabilities**:
     - K is the number of classes.
     - The output is a probability distribution over the classes.
  3. It **predicts** the class with the **highest probability**:
- Training the Model
  - The model is trained to **maximize the probability** of the correct class.
  - It uses the **cross-entropy loss function**:

        - =1 if example belongs to class k, else 0.
        - This function penalizes the model when it assigns **low probability** to the correct class.
        - When K=2, this reduces to the familiar **log loss** used in binary logistic regression.
- Key Tip
    - Softmax is good for **mutually exclusive classes** (e.g., flower types), but **not** for multi-label problems (like detecting multiple objects in one image).
- Cross Entropy in Machine Learning
    - Used as the **loss function** for classification tasks.
    - Penalizes wrong class probability predictions.
    - Especially common in **softmax regression** and **neural networks**.
- Gradient of Cross Entropy
    - Helps in **training the model** using gradient descent:
    - Compute gradient per class → update weights → repeat.
- **Softmax Regression with Scikit-Learn**
    - Automatically used when there are **more than 2 classes**.
    - Uses **LogisticRegression** with `solver="lbfgs"` (default).
    - Regularized using L2 by default (controlled by `C`).
    - **Example: Classify Iris Flowers**

```
X = iris.data[["petal length (cm)", "petal width (cm)"]].values
y = iris["target"]
X_train, X_test, y_train, y_test = train_test_split(X, y,
random_state=42)
softmax_reg = LogisticRegression(C=30, random_state=42)
softmax_reg.fit(X_train, y_train)
```

    - Prediction Example:

```
softmax_reg.predict([[5, 2]])  # → array([2])
softmax_reg.predict_proba([[5, 2]])  # → [[0.  , 0.04, 0.96]]
```

- **Visualization**

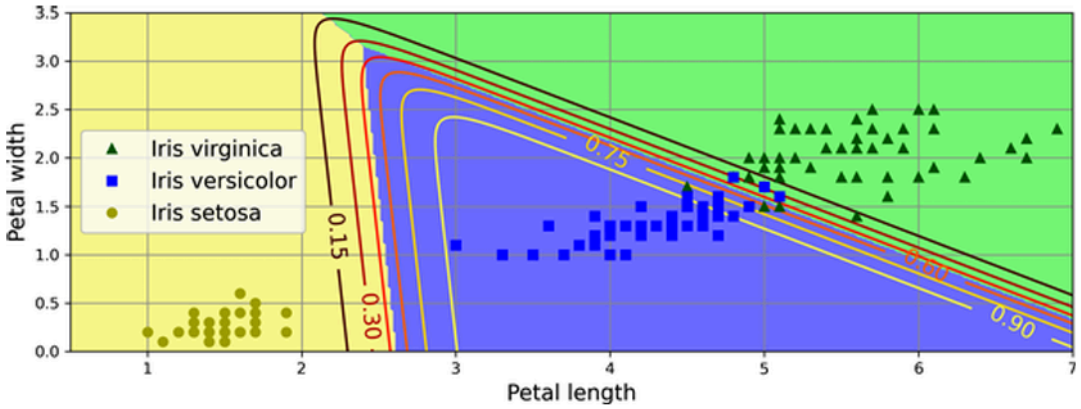


Figure 4-25. Softmax regression decision boundaries

- Softmax regression creates **linear decision boundaries** between classes.
- Curved lines represent **equal probability contours**.
- At the center where all three classes meet → model gives ~33% to each class.

Resources :

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Related notes :

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References :

- **Internal :**
  -
  -
  -
- **External :**
- notebook of the chapter
- hegab videos

- the book