



# Patterns, Predictions, and Actions

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STAT 499: DRP

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# Content

1. Fundamentals of Prediction

2. Risk Minimization

3. Dataset

4. Gradient Descent

5. SGD

6. Generalization

# 1. Fundamentals of Prediction

- Attributes/covariates:  $X \in \mathcal{X}$
- Label/target:  $Y \in \mathcal{Y}$
- Function/predictor:  $f(x)$
- Loss:  $l(y, f(x))$ 
  - Eg. 0, 1 - loss, Brier loss
- Risk:  $R(f) = E[l(y, f(x))]$ 
  - Eg. in regression case  $R(f) = \text{MSE} = E[(Y - f(x))^2]$
- Goal:  $\arg \min_f R[f]$

## 2. Risk Minimization

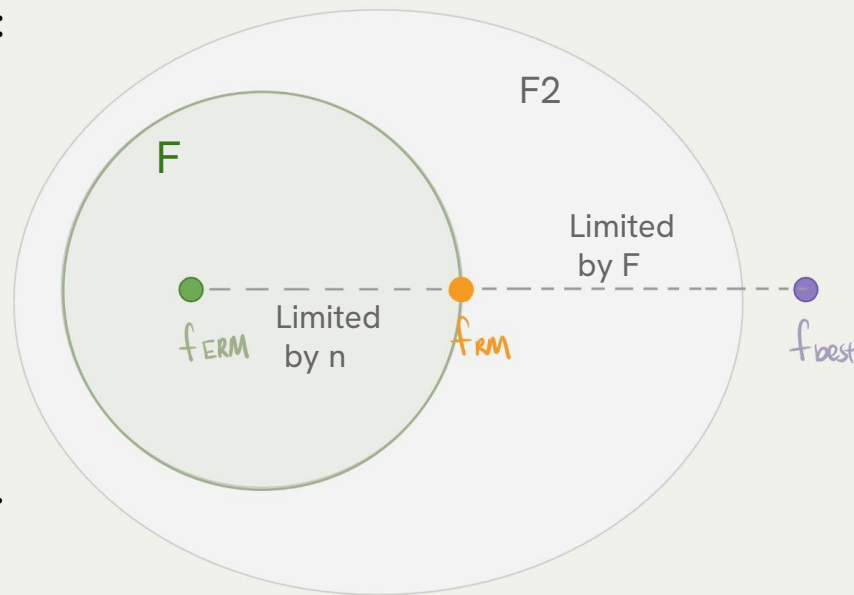
- To find risk need to choose two functions:

1. loss function

$$\text{(e.g. } l(y, f(x)) = (Y - f(x))^2 \text{)}$$

2. prediction function  $f(x)$

- Risk Minimization:  $\arg \min_{f \in F} R[f]$ 
  - need to define a function class  $F$
  - e.g. simple, multiple linear, logistic, etc.
- Empirical risk minimization (ERM)



### 3. Dataset: `load\_breast\_cancer`

- ``sklearn.datasets.load_breast_cancer``
- Breast cancer Wisconsin dataset
- Binary classification
- $n = 569$
- 30 features/covariates
- Loss: MSE,
- F: multiple linear regression

# Approaches

1. Assume **normal distribution**
  - a. Compare which class the given sample is more likely to belongs
2. OLS Analytical solution  $\beta^* = (X^T X)^{-1} X^T Y$
3. Gradient descent
4. SGD and variations

```
def predict_label(x_i, mu_0, sigma_0, mu_1, sigma_1):  
    p_0 = norm.pdf(x_i, loc=mu_0, scale=sigma_0)  
    p_1 = norm.pdf(x_i, loc=mu_1, scale=sigma_1)  
    predicted_label = np.where(p_1 > p_0, 1, 0)  
    return predicted_label
```

0.0s

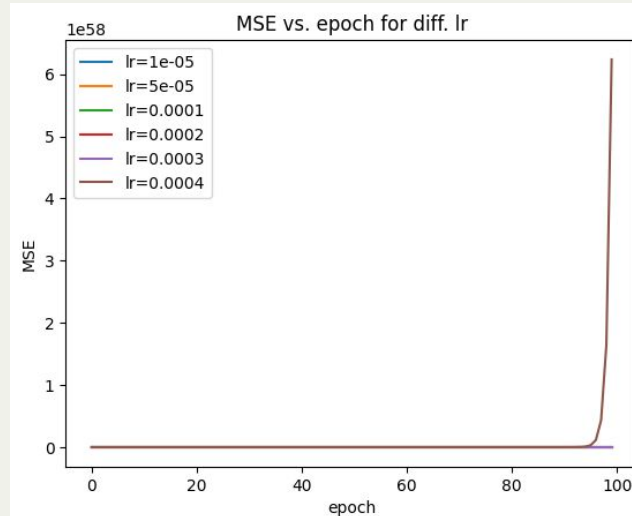
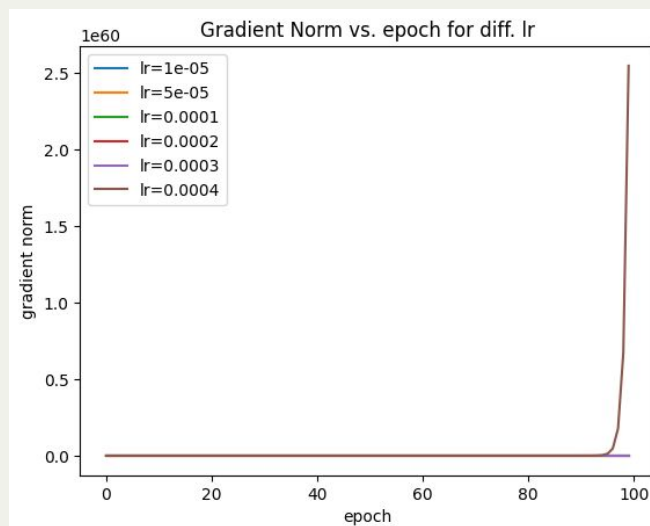
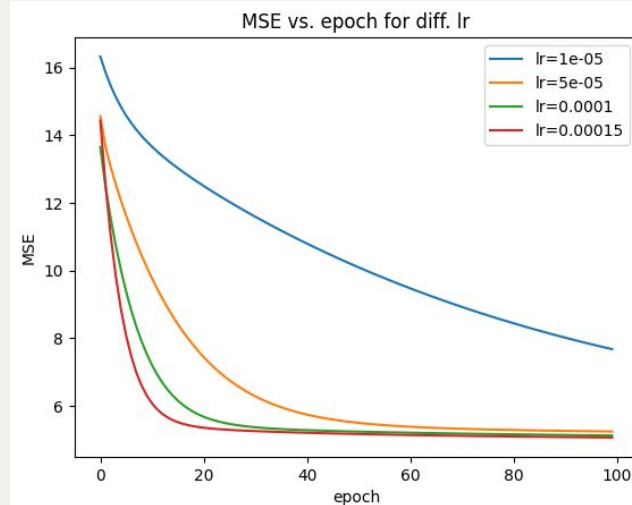
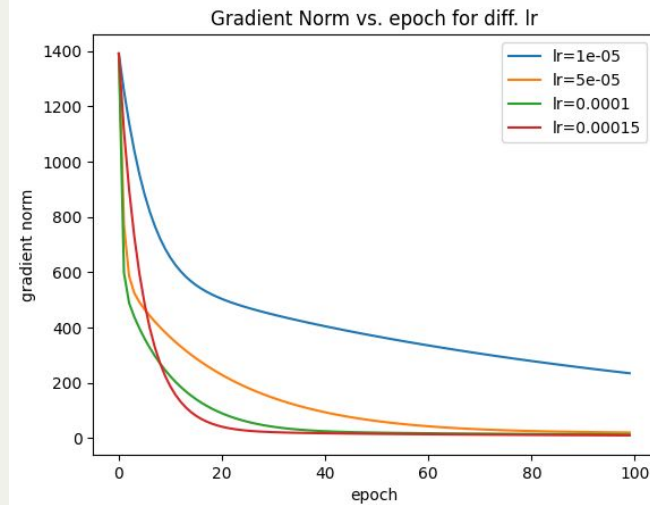
training accuracy: 87.25%

training accuracy: 87.47%

## 4. Gradient Descent - Full-batch

- $\min_{\beta} ||Y - X\beta||^2 = \min_{\beta} Y^T Y - 2X^T Y \beta + \beta^T X^T X \beta$
- $\Phi(w) = w^T Q w - P^T w + r$ 
  - where  $P = 2X^T Y$  and  $Q = 2X^T X$
- $\nabla \Phi(w) = Qw - P$
- Goal: find optimal  $w^*$  st.  $\nabla \Phi(w^*) = 0$
- Gradient Descent:  $w_{t+1} = w_t - \alpha \nabla \Phi(w_t)$
- learning rate  $\alpha$

# Gradient Norm & MSE

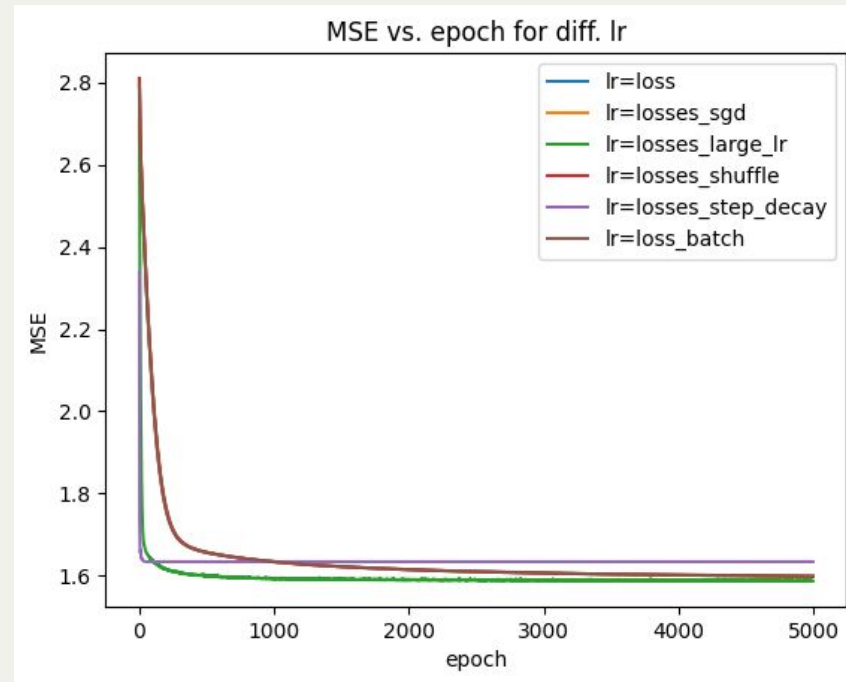
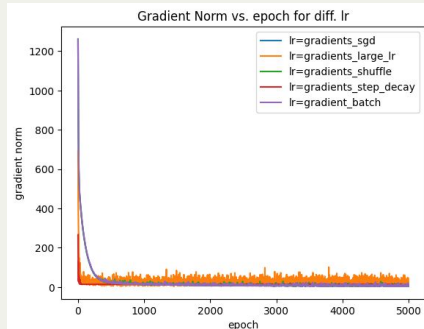
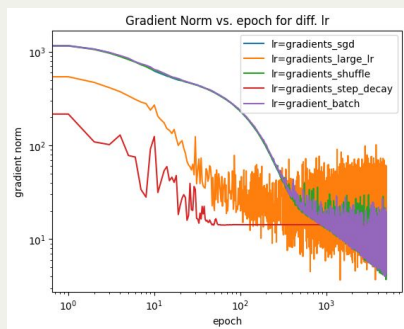
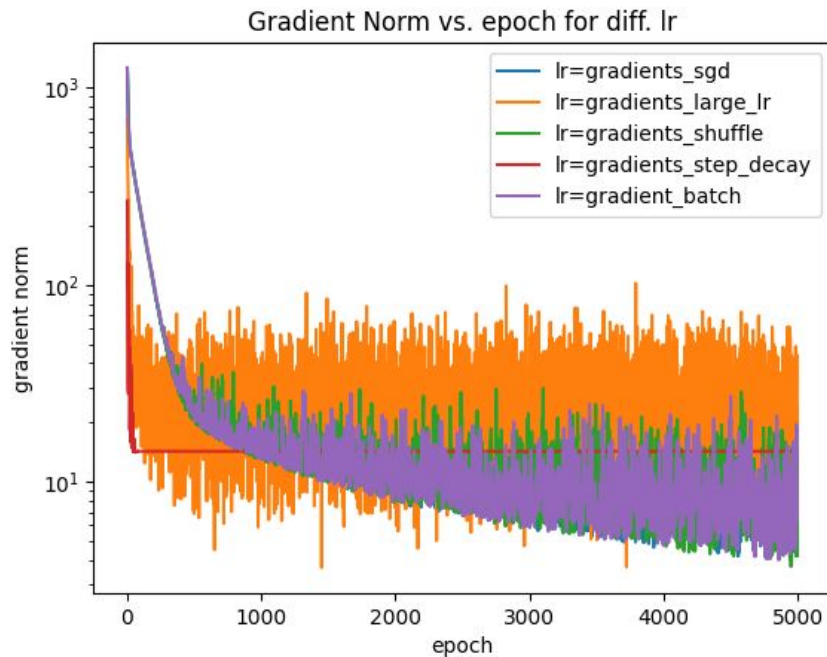




## 5. SGD

- $w_{t+1} = w_t - \alpha_t \nabla l_{w_t}(f(x_i), y_i)$ 
  - $i$  is random, i.e. a random sample select from the dataset
  - update weight after each point,  $n$  \* epoch updates
- Mini-batch: update the weight after  $m$  examples,  
 $\frac{n}{m}$  \* epoch updates
  - $w_{k+1} = w_k - \alpha_k \frac{1}{m} \sum_{j \in \text{batch}_k} \nabla l_{w_k}(f(x_j), y_j)$
- Shuffling: sampling each gradient with replacement
- Step decay: suppose  $\alpha_0 = 0.001$ ,  $\alpha_t = \alpha_0 \gamma^t$ ,  $\gamma = 0.9$

# Gradient Norm & MSE



## 6. Generalization

- $\hat{f} = \arg \min_{f \in F} R_s(f)$  via optimization
- Goal:  $f^* = \arg \min_{f \in F} R(f)$  population
- $R(\hat{f}) = R_s(\hat{f}) + (R(\hat{f}) - R_s(\hat{f}))$



Generalization Gap

Thank you!

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Q&A

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