# Linear Regression

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# 1 Discrete to Continuous Labels

From classification to regression

## 1.1 Task

Given $X \in \mathcal{X}$, predict $Y \in \mathcal{Y}$, Construct prediction rule $f : \mathcal{X} \to \mathcal{Y}$

### 1.2 Performance Measure

- Quantifies knowledge gained.
- Measure of closeness between true label Y and prediction f(X)
  - 0/1 lose:$loss(Y, f(X)) = 1_{f(X)\neq Y}$. Risk: probability of error
  - square loss: $loss(Y, f(X)) = (f(X) - Y)^2$. Risk: mean square error
- How well does the predictor perform on average?

$$Risk\ R(f) = \mathbb{E}[loss(Y, f(X))],\ (X, Y) \sim P_{XY}$$

### 1.3 Bayes Optimal Rule

- ideal goal: Construct prediction rule $f^* : \mathcal{X} \to \mathcal{Y}$

$$f^* = \arg\min_f E_{XY}[loss(Y, f(X))]$$

  (Bayes optimal rule)
- Best possible performance:

$$\forall f,\ R(f^*) \leq R(f)$$

  (Bayes Risk)

Problem: $P_{XY}$ is unknown.
Solution: Training data provides a glimpse of $P_{XY}$

$$\text{(observed) } \{(X_i, Y_i)\} \sim_{i.i.d} P_{XY} \text{ unknown}$$

## 2 Macine Learning Algortihm

- Model based approach: use data to learn a model for $P_{XY}$
- Model-free approach: use data to learn mapping directly

### 2.1 Empirical Risk Minimization (model-free)

- Optimal predictor:

$$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

- Empirical Minimizer:

$$\hat{f}_n = \arg\min_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^{n}(f(X) - Y)^2$$

$\mathcal{F}$ is the class of predictors:

- Linear
- Polynomial
- Nonlinear

# 3 Linear Regression

$$f(\vec{X}) = \sum_{i=0}^{p} \beta_0 X^i = \vec{X}^T \vec{\beta},\ where\ X^0 = 1,\ \vec{\beta} = [\beta_0, \ldots, \beta_p]^T$$

$$\hat{\vec{\beta}} = \arg\min_{\vec{\beta}} (A^T\vec{\beta} - \vec{Y})^T (A^T\vec{\beta} - \vec{Y}),\ where\ A = [\vec{X}_1, \ldots, \vec{X}_n]$$

$$J(\beta) = (A^T\vec{\beta} - \vec{Y})^T (A^T\vec{\beta} - \vec{Y})$$

$$\begin{aligned}
\frac{\partial J(\vec{\beta})}{\partial \vec{\beta}} &= \frac{\partial (A^T\vec{\beta}-\vec{Y})^T(A^T\vec{\beta}-\vec{Y})}{\partial \vec{\beta}} \\
&= \frac{\partial (\vec{\beta}^T AA^T\vec{\beta} - \vec{\beta}^T A\vec{Y} - \vec{Y}^T A^T\vec{\beta} + \vec{Y}^T\vec{Y})}{\vec{\beta}} \\
&= (AA^T + (AA^T)^T)\vec{\beta} - A\vec{Y} - A\vec{Y} \\
&= 2AA^T\vec{\beta} - 2A\vec{Y} = 0 \\
&\Rightarrow AA^T\vec{\beta} = A\vec{Y} \\
&\Rightarrow \hat{\vec{\beta}} = (AA^T)^{-1}A\vec{Y},\ \text{if } AA^T \text{ is invertible}
\end{aligned}$$

## 3.1 Gradient Descent

Even when $AA^T$ is invertible, might be computationally expensive if $A$ is huge; however, $J(\vec{\beta})$ is convex[1] in $\beta$.
Minimum of a convex function can be reached by gradient descent algorithm:

- Initialize: pick $\vec{w}$ at random
- Gradient:
$$\nabla_{\vec{w}} l(\vec{w}) = [\frac{\partial l(\vec{w})}{\partial w_0}, \ldots, \frac{\partial l(\vec{w})}{\partial w_d}]^T$$
- Update rule:
$$\Delta \vec{w} = \eta \nabla_{\vec{w}} l(\vec{w})$$
,
$$w_i^{t+1} \leftarrow w_i^t - \eta \frac{\partial l(\vec{w})}{\partial w_i}|_t$$
- Stop: when some criterion met $\frac{\partial l(\vec{w})}{\partial w_i}|_t < \epsilon$

## 3.2 If $AA^T$ is not invertible

$Rank(AA^T)$ = number of non-zero eigenvalues of $AA^T$ = number of non-zero singular values of A $\leq \min(n,p)$ since $A$ is $n \times p$

$$A = U\Sigma V^T \Rightarrow AA^T = U\Sigma^2 U^T \Rightarrow AA^T U = U\Sigma^2$$

### 3.2.1 Regularized Leasts Squares

Ridge Regression (L2 penalty)

$$\begin{aligned}
\hat{\vec{\beta}}_{MAP} &= \arg\min_{\vec{\beta}} (A^T\vec{\beta} - \vec{Y})^T (A^T\vec{\beta} - \vec{Y}) + \lambda \vec{\beta}^T\vec{\beta} \quad (\lambda \geq 0) \\
&= (AA^T + \lambda I)^{-1} A\vec{Y}
\end{aligned} \tag{1}$$

$(AA^T + \lambda I)$ is invertible if $\lambda > 0$. Proof:

- the symmetric matrix $AA^T$ is positive-semidefinite matrix, because a matrix is positive-semidefinite iff it arises as the Gram matrix of some set of vectors[2].

[1] A function is called convex if the line joining any two points on the function does not go below the function on the interval formed by these two points.

[2] In contrast to the positive-definite case, these vectors need not be linearly independent.

- $\therefore \forall\lambda > 0 \; and \; \vec{x} \neq \vec{0}$,
$$\vec{x}^T(AA^T)\vec{x} = (A^T\vec{x})^T(A^T\vec{x}) \geq 0$$
$$\vec{x}^T(AA^T + \lambda I)\vec{x} = \vec{x}^T(AA^T)\vec{x} + \lambda\vec{x}^T\vec{x} > 0$$
- $\therefore (AA^T + \lambda I)$ is positive definite.
- $\therefore$ the eigenvalues of $B = (AA^T + \lambda I)$ are all positive.
$$B\vec{v} = \lambda\vec{v} \Rightarrow \vec{v}^T B\vec{v} = \lambda > 0$$
- $\therefore (AA^T + \lambda I)$ is invertible if $\lambda > 0$

#### 3.2.2 Understanding Regularized Least Squared

Why we need constraints: r equations, p unknowns - underdetermined system of linear equations.

$$\min_{\vec{\beta}} J(\beta) + \lambda pen(\vec{\lambda})$$

- Ridge Regression: $pen(\beta) = ||\beta||_2^2$
- Lasso Regression: $pen(\beta) = ||\beta||_1$. No closed form solution, but can optimize using sub-gradient descent.
- $pen(\beta) = ||\beta||_0 = \sum 1_{\beta_i \neq 0}$

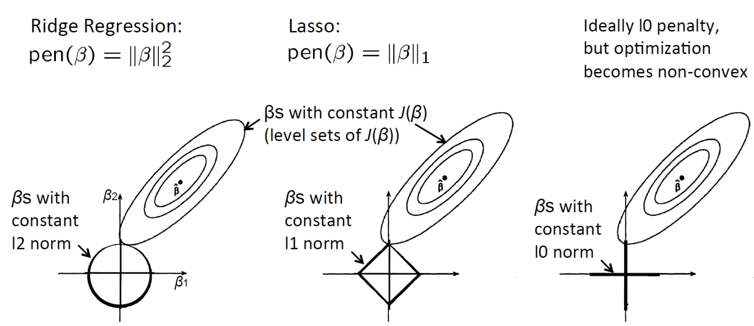



Figure 1: For Lasso regression, results are in sparse solution - vector with more zero coordinates. Good for high-dimenstional problems - don't have to store all coordinates, interpretable solution!

Matlab code:

```
[B, FitInfo] = lasso(X,Y,Name,Value)
```

- X: Numeric matrix with n rows and p columns. Each row represents one observation, and each column represents one predictor (variable).
- Y: Numeric vector of length n, where n is the number of rows of X. Y(i) is the response to row i of X.
- 'Alpha': Scalar value from 0 to 1 (excluding 0) representing the weight of lasso (L1) versus ridge (L2) optimization. Alpha = 1 represents lasso regression, Alpha close to 0 approaches ridge regression, and other values represent elastic net optimization. See Definitions. Default: 1

### 3.3 Regularized Least Squares - Connection to MLE and MAP (Model-based Approaches)

#### 3.3.1 Least Squares and M(C)LE (Maximum Conditional Likelihood Estimator)

$$Y = f^*(X) + \epsilon = X\beta^* + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \sigma^2 I) \ \ Y \sim \mathcal{N}(X\beta^*, \sigma^2 I)$$
$$\hat{\beta}_{MLE} = \arg\max_{\beta}(\log p(\{Y_i\}|\beta, \sigma^2, \{X_i\})) = \arg\min_{\beta} \sum_i (X_i\beta - Y_i)^2$$

- Model parameters: $\beta, \sigma^2$
- Conditional log likelihood: $\log p(\{Y_i\}|\beta, \sigma^2, \{X_i\})$

Least Square Estimator is same as Maximum Conditional Likelihood Estimator under a Gaussian model.

#### 3.3.2 Regularized Least Squares and M(C)AP (Maximum Conditional A Prior Estimator)

If $AA^T$ is not invertible.

$$Y = f^*(X) + \epsilon = X\beta^* + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \sigma^2 I) \ \ Y \sim \mathcal{N}(X\beta^*, \sigma^2 I)$$

(1) Gaussian prior:

$$\beta \sim \mathcal{N}(0, \tau^2 I) \ \ p(\beta) \propto \exp(-\beta^T\beta/2\tau^2)$$
$$\hat{\beta}_{MAP} = \arg\max_{\beta} \log p(\{Y_i\}|\beta, \sigma^2, \{X_i\}) + \log p(\beta) = \arg\min_{\beta} \sum_i (X_i\beta - Y_i)^2 + \lambda(\sigma^2, \tau^2)||\beta||_2^2$$

(2) Laplace prior:

$$\beta \sim \mathit{Laplace}(0, t) \ \ p(\beta_i) \propto \exp(-|\beta_i|/t)$$
$$\hat{\beta}_{MAP} = \arg\max_{\beta} \log p(\{Y_i\}|\beta, \sigma^2, \{X_i\}) + \log p(\beta) = \arg\min_{\beta} \sum_i (X_i\beta - Y_i)^2 + \lambda(\sigma^2, \tau^2)||\beta||_1$$

- Model parameters: $\beta, \sigma^2$
- Conditional log likelihood: $\log p(\{Y_i\}|\beta, \sigma^2, \{X_i\})$
- Log prior: $\log p(\beta)$

# 4 Polynomial Regression

- Univariate: $f(X) = \sum \beta_i X^i = [1, X, X^2, \dots, X^m]^T\beta$

$$\hat{\beta} = (AA^T)^{-1}AY \ \mathit{or} \ (AA^T + \lambda I)^{-1}AY$$

- Multivariate: $f(X) = \sum_i \beta_i X^{(i)} + \sum_{i,j} \beta_{i,j} X^{(i)}X^{(j)} + \sum_{i,j,k} \beta_{i,j,k} X^{(i)}X^{(j)}X^{(k)} + \dots$

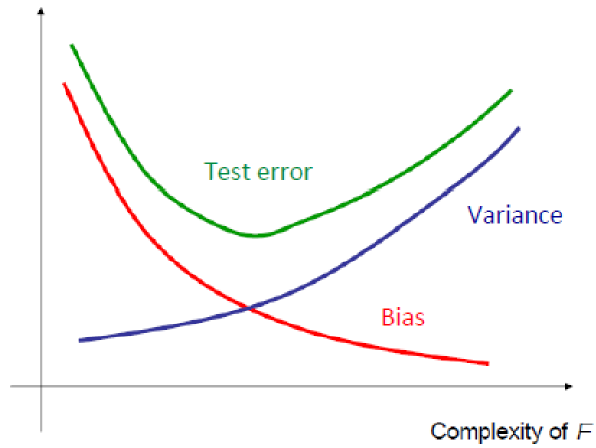
## 4.1 Bias - Vairance Tradeoff

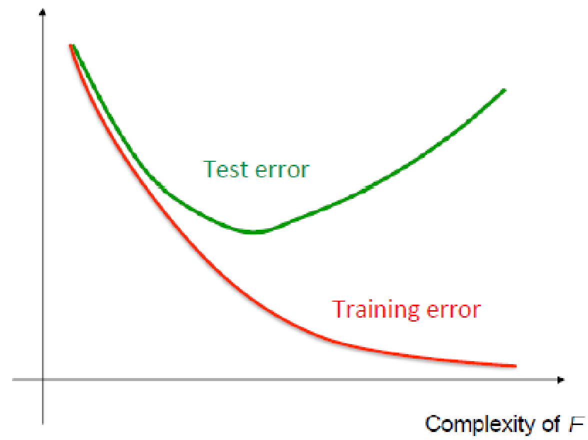
- Large bias, small variance: poor approximation but robust/stable
- Small bias, large variance: good approximation but unstable

Bias-Variance Decomposition:

$$E[(f(X) - f^*(X))^2] = Bias^2 + Variance$$

- $Bias = E[f(X)] - f^*(X)$: How far is the model from best model.
- $Variance = E[(f(X) - E[f(X)])^2]$: How variable is the model.






# 5 Regression with Basis Functions or Nonlinear Features

$$f(X) = \sum_i \beta_i \phi_i(X)$$