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Feature Selection

Data Mining 11 (データマイニング)

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Today's Outline

- Today's topic is feature selection
  - Find relevant variables from datasets
- Feature selection detects variables, or features, that are associated with the target variable from the set of all variables in a given dataset
  - The target variable can be binary (0 and 1 for cases and controls) in a case-control study or continuous

Variable Ranking (Filter Method)

1. Measure the degree of association between the target variable and each variable by some scoring method
   - Pearson's correlation coefficient
   - Mutual information
2. Rank variables using the score

- The above two-step procedure is called the filter method

Pearson's Correlation Coefficient

- (Pearson's) correlation coefficient ρ measures the linear association between two variables
  - The larger the absolute value $|\rho|$ is, the stronger the association is
  - $\rho > 0$ means the positive correlation, $\rho < 0$ the negative correlation
- ρ between two random variables X and Y is defined as

$$\rho = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} = \frac{\mathbf{E}\Big[(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])\Big]}{\sqrt{\mathbf{E}\Big[(X - E[X])^2\Big]\,\mathbf{E}\Big[(Y - E[Y])^2\Big]}}$$

  - σ_{XY} is the covariance, σ_X is the standard deviation
  - $\mathbf{E}[X]$ is the expectation

Sample Correlation Coefficient

- Given a dataset (sample) $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$, the sample correlation coefficient r is computed as

$$r = \frac{\sum_{i=1}^{N}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \overline{x})^2 \sum_{i=1}^{N}(y_i - \overline{y})^2}},$$

$$\overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i, \quad \overline{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$$

Properties of Correlation Coefficient

- $-1 \leq \rho \leq 1$ and 1, -1 are the strongest correlation
- X and Y are independent $\Rightarrow \rho(x) = 0$
  - X and Y are (statistically) independent if

    $P(X \cup Y) = P(X)P(Y)$

    and denoted by $X \perp\!\!\!\perp Y$
- However, [$\rho(x) = 0 \Rightarrow X$ and Y are independent] does not hold
  - $\rho(x)$ can be 0 for nonlinear association

Mutual Information

- For a pair of discrete random variables X and Y, the mutual information is defined as

$$I(X, Y) = \sum_{x \in X} \sum_{y \in Y} p(x, y) \log \left(\frac{p(x, y)}{p(x)p(y)} \right)$$

  - $p(x, y)$: joint probability, $p(x)$ and $p(y)$: marginal probability
- Properties:
  - $I(X, Y) \geq 0$
  - $I(X, Y) = H(X) + H(Y) - H(X, Y) = H(X) - H(Y \mid X)$
    - $H(X)$ is the entropy: $-\sum_{x \in X} p(x) \log p(x)$
    - $H(X, Y)$ is the joint entropy: $-\sum_{x \in X} \sum_{y \in Y} p(x, y) \log p(x, y)$

Properties of Mutual Information

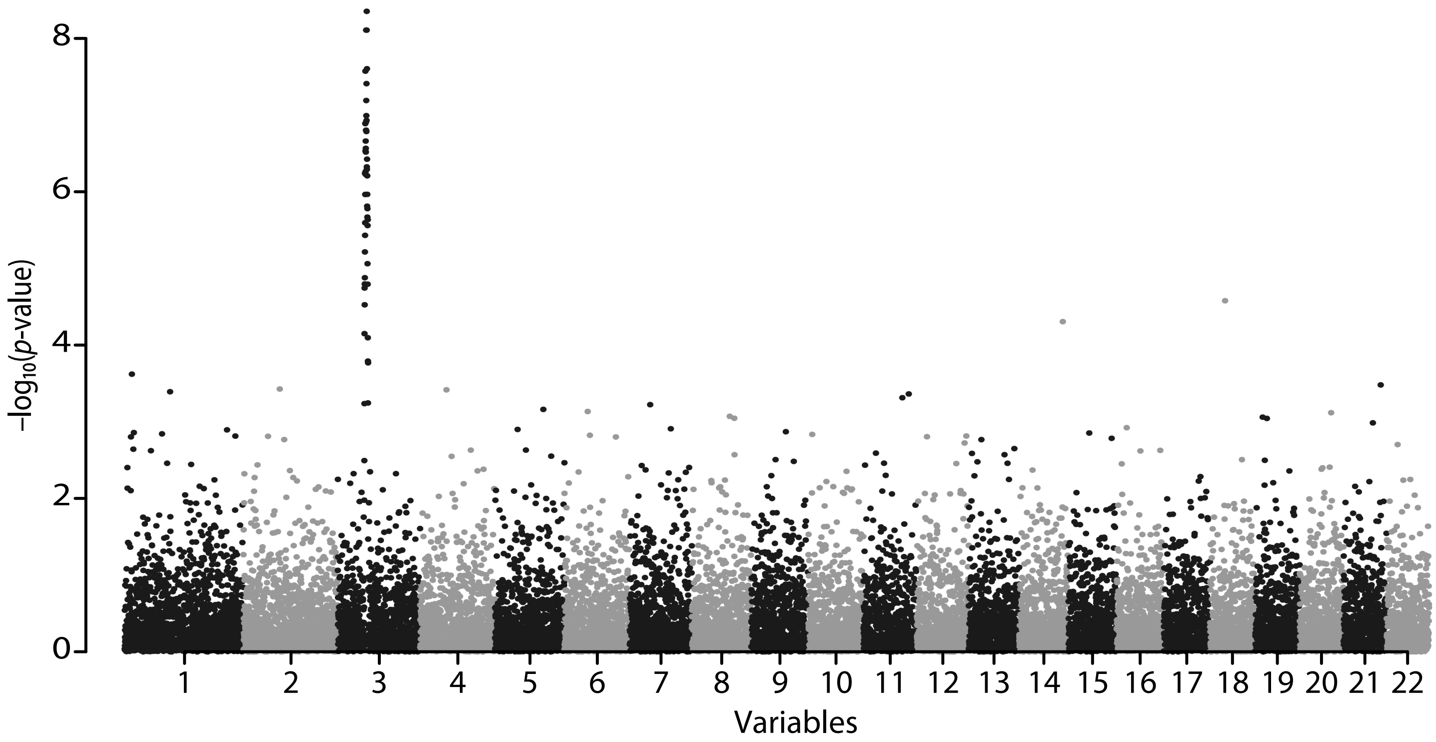
- **Pros:**
  - The mutual information can measure both linear and nonlinear associations
    - X and Y are independent $\iff I(X,Y) = 0$
- **Cons:**
  - Additional discretization is needed to estimate the mutual information for continuous variables
  - Not normalized in the original form, but can be normalized by

$$I^*(X,Y) = \frac{I(X,Y)}{\sqrt{H(X)H(Y)}}$$

Computing the *p*-value

- p-value shows the probability of getting the dataset with assuming that there is no association between variables
  - Often used in science, e.g. biology
- Permutation test can be used to compute the p-value
  (i) Compute the association score s of the given dataset
  (ii) Repeat the following h times and get h scores $s_1, s_2, \dots, s_h$:
    a. Fix x and permute indices of y
    b. Compute the score using the permuted indices
  (iii) The p-value $= |\{i \in [h] \mid s_i > s\}| \,/\, h$

Manhattan Plot for Visualization



Properties of Filter Method

- **Pros:**
  - Easy to use
  - Easy to understand
- **Cons:**
  - Redundant features might be selected as interactions between variables are not considered
    - If a dataset contains exactly the same variables that have the strong association with the target variable, both variables are selected

Wrapper Method

- A wrapper method repeats to construct a classifier for each subset of variables
  (i) Given a dataset with n variables $X^1, X^2, \dots, X^n$ and a target variable Y
  (ii) Repeat the following for every subset $I \subseteq [n]$
    a. Construct a subset of the dataset using only variables in I
    b. Apply classification and measure the goodness (e.g. MSE)
  (i) Choose the best subset
- It is computationally too expensive if n is large

Embedded Method

- Variables are automatically selected during the process of learning a prediction model from a dataset
- The representative method: the Lasso
  - It learns a linear prediction model, where a set of variables, which receive nonzero coefficients, is automatically selected in the learning process by regularizing the number of variables
  - The joint additive effect of selected variables maximizes the prediction accuracy of the model

The Lasso

- The Lasso is the following optimization problem

$$\min_{\boldsymbol{w}, \boldsymbol{w}_0} \frac{1}{N} \sum_{i=1}^{N} \Big(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle - w_0 \Big)^2 \quad \text{s.t. } \|\boldsymbol{w}\|_1 \leq t$$

  - $\|\boldsymbol{w}\|_1 = \sum_{j=1}^{n} |w^j|$ (ℓ_1-norm)
  - Minimizing squared error loss with the constraint
- The solution typically has many of the w^j equal to zero
  - $\{j \in [n] \mid w^j \neq 0\}$, called the active set, is considered to be the set of selected variables

The Lasso

- More convenient Lagrange form of the Lasso;

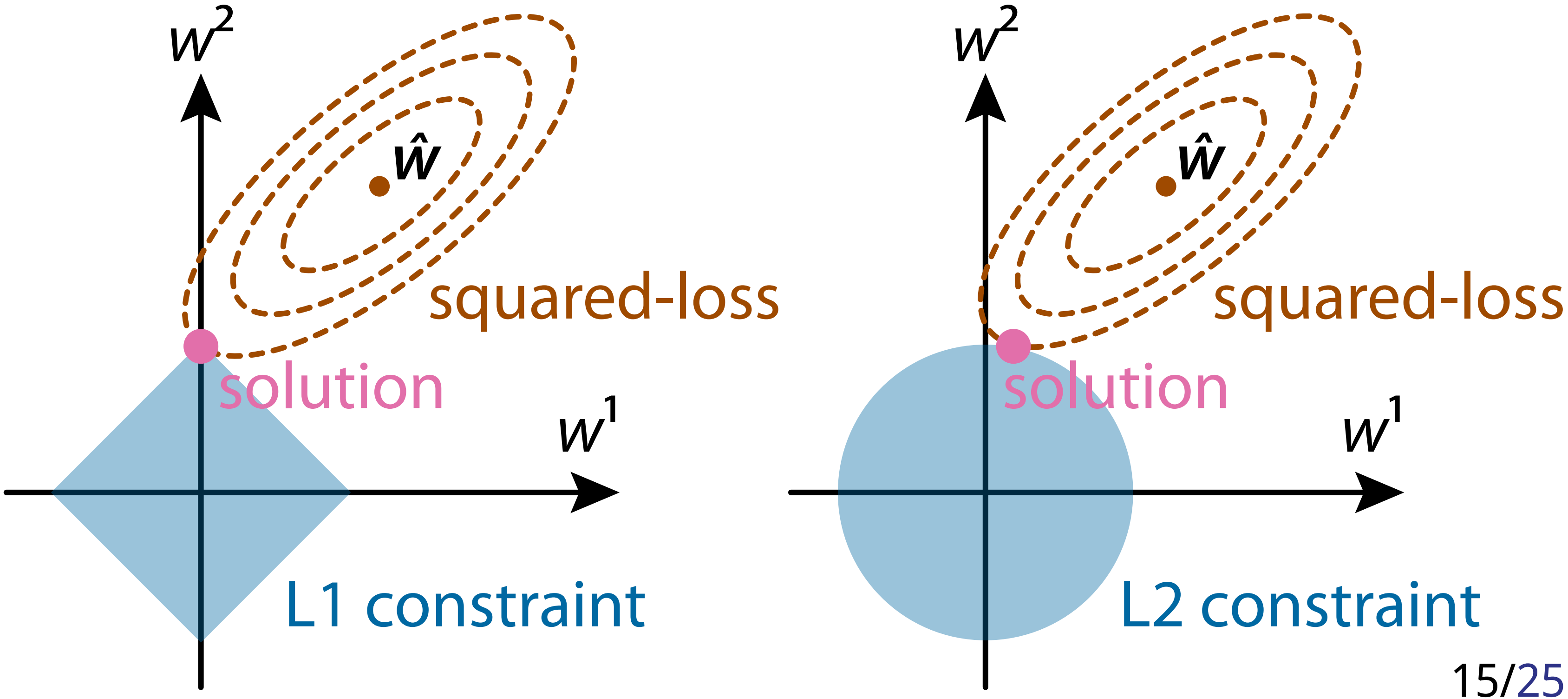
$$\min_{\boldsymbol{w}, w_0} \frac{1}{2N} \sum_{i=1}^{N} \Big(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle - w_0 \Big)^2 + \lambda ||\boldsymbol{w}||_1$$

- If we center the dataset beforehand, it can be written as

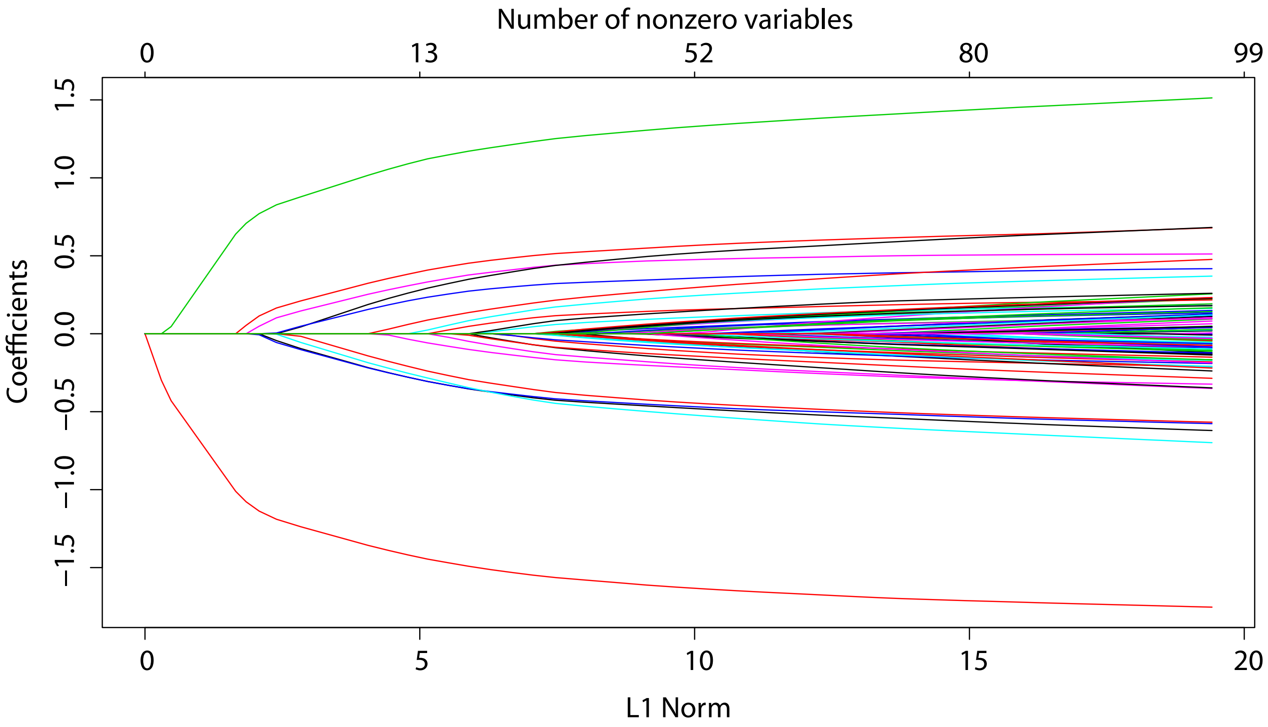
$$\min_{\boldsymbol{w}} \frac{1}{2N} \sum_{i=1}^{N} \Big(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle \Big)^2 + \lambda ||\boldsymbol{w}||_1,$$

$$\min_{\boldsymbol{w}} \frac{1}{2N} ||\boldsymbol{y} - X\boldsymbol{w}||_2^2 + \lambda ||\boldsymbol{w}||_1,$$

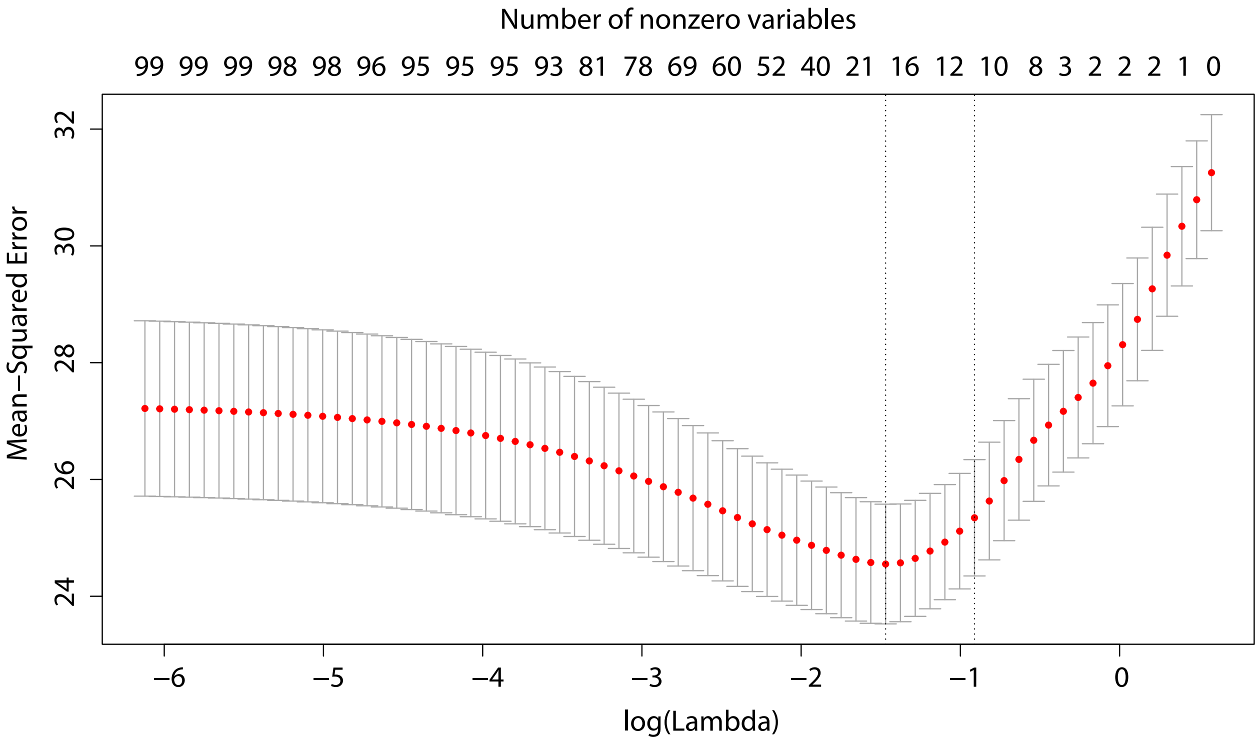
Lasso Constraint



Regularization Path ($N = 1000$, $n = 100$)



MSE ($N = 1000$, $n = 100$)



Fitting of the Lasso

- Solution of the Lasso problem satisfies the subgradient condition:

$$-\frac{1}{n}\langle \boldsymbol{x}^j, \boldsymbol{y} - X\hat{\boldsymbol{w}}\rangle + \lambda s^j = 0, \quad j = 1, 2, \dots, n$$

  - $\boldsymbol{x}^j = (x_1^j, x_2^j, \dots, x_N^j) \in \mathbb{R}^N$
  - $s_j = \text{sign}(\hat{w}^j)$ if $\hat{w}^j \neq 0$ and $s_j \in [-1, 1]$ if $\hat{w}^j = 0$

- Thus we have

$$\begin{cases} -\frac{1}{n}\left|\langle \boldsymbol{x}^j, \boldsymbol{y} - X\hat{\boldsymbol{w}}\rangle\right| = \lambda, & \text{if } w^j \neq 0, \\ -\frac{1}{n}\left|\langle \boldsymbol{x}^j, \boldsymbol{y} - X\hat{\boldsymbol{w}}\rangle\right| \leq \lambda, & \text{if } w^j = 0, \end{cases}$$

- $\hat{\boldsymbol{w}}$ is a piecewise-linear function w.r.t. $\lambda \to$ LAR algorithm

Algorithm 1: Least Angle Regression

```
LAR($X$, $\boldsymbol{y}$)
    Standardize $X$ (mean zero, unit $\ell 2$ norm)
    $\boldsymbol{r}_0 = \boldsymbol{y} - \overline{\boldsymbol{y}}$, $\boldsymbol{w}_0 \leftarrow (0, 0, \dots, 0)$
    Find $\boldsymbol{x}^j$ which has the largest correlation $|\langle \boldsymbol{x}^j, \boldsymbol{r}_0 \rangle|$
    $\lambda_0 \leftarrow (1/N)|\langle \boldsymbol{x}^j, \boldsymbol{r}_0 \rangle|$; $A \leftarrow \{j\}$; $X_A \leftarrow X$ with only $A = \{j\}$
    foreach $k \in \{1, 2, \dots, K = \min\{N-1, n\}\}$ do
        LAREACH($X$, $\boldsymbol{y}$, $A$, $\lambda_{k-1}$, $\boldsymbol{r}_{k-1}$, $\boldsymbol{w}_{k-1}$)
```

Algorithm 2: Least Angle Regression

LAREach(X, $\boldsymbol{y}$, A, λ_{k-1}, $\boldsymbol{r}_{k-1}$, $\boldsymbol{w}_{k-1}$)

- $\delta \leftarrow (1/n\lambda_{k-1})(X_A^T X)^{-1} X_A^T \boldsymbol{r}_{k-1}$
- $\Delta \leftarrow (0, 0, \dots, 0)$; $\Delta_A \leftarrow \delta$
- $\boldsymbol{w}(\lambda) \leftarrow \boldsymbol{w}_{(k-1)} + (\lambda_{k-1} - \lambda)\Delta$ for $0 < \lambda \leq \lambda_{k-1}$
- $\boldsymbol{r}(\lambda) \leftarrow \boldsymbol{y} - X\boldsymbol{w}(\lambda) = \boldsymbol{r}_{k-1} - (\lambda_{k-1} - \lambda) X_A \delta$
- Decrease λ and find $\ell \notin A$ that first achieves $(1/N)|\langle \boldsymbol{x}^j, \boldsymbol{r}(\lambda) \rangle| = \lambda$
- $A \leftarrow A \cup \{\ell\}$; $\boldsymbol{w}_k \leftarrow \beta(\lambda_k)$; $\boldsymbol{r}_k \leftarrow \boldsymbol{y} - X\boldsymbol{w}_{(k)}$

Dimension Reduction

- Dimension reduction also reduces the number of variables
- Variables are not directly selected but transformed into principal variables
- t-SNE (t-distributed stochastic neighbor embedding) is recently becoming a popular method and often used to visualize a multi-dimensional dataset (van der Maaten and Hinton, 2008)
  - This can be used for visualization

t-SNE

- Given a dataset $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$, define $p_{j|i}$ for each $i, j \in [N]$ as

$$p_{j|i} = \frac{\exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_k\|^2 / 2\sigma_i^2\right)}$$

  - σ_i is the variance of the Gaussian
  - $p_{i|i} = 0$
  - We also use $p_{ij} = (p_{j|i} + p_{i|j})/2N$
- **Goal:** Find low-dimensional $\boldsymbol{y}_1, \boldsymbol{y}_2, \dots, \boldsymbol{y}_N$ of the original $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N$ with keeping the proxy between points

How to Set Variance

- Given the perplexity as a parameter, which is defined as

  $\text{Perp}(P_i) = 2^{H(P_i)}$

  for a distribution P_i and its entropy $H(P_i)$ such that

  $$H(P_i) = -\sum_j p_{j|i} \log p_{j|i}$$

- For each $i \in [N]$, find σ_i^2 that satisfies the given perplexity
- In practice, the perplexity from 5 to 50 is recommended

t-SNE Formulation

- For low-dimensional $\boldsymbol{y}_i, \boldsymbol{y}_j$ of $\boldsymbol{x}_i, \boldsymbol{x}_j$,

$$q_{ij} = \frac{\left(1 + \|\boldsymbol{y}_i - \boldsymbol{y}_j\|^2\right)^{-1}}{\sum_k \sum_{l \neq k} \left(1 + \|\boldsymbol{y}_k - \boldsymbol{y}_l\|^2\right)^{-1}}$$

- The cost C is the KL divergence: $C = D_{\mathrm{KL}}(P, Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$
- t-SNE finds low-dimensional $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_N$ that minimizes the cost C
  - The gradient descent can be used for optimization

$$\frac{\partial C}{\partial \boldsymbol{y}_i} = 4 \sum_j (p_{ij} - q_{ij})(\boldsymbol{y}_i - \boldsymbol{y}_j) \left(1 + \|\boldsymbol{y}_i - \boldsymbol{y}_j\|^2\right)^{-1}$$

Summary

- Feature selection can find relevant variables (features)
  - Filter method, wrapper method, embedded method
- The Lasso is the representative embedded method
- t-SNE is the representative dimension reduction method