Regression

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Linear regression

- Linear model $f(x,\beta)=x^T\beta=\sum_{i=1}^D \beta_i x^i$
- Define $X\in\mathbb{R}^{NxD}, \{X\}_{ij}$ defines the j-th feature of i-th object, $Y\in\mathbb{R}^n$, $\{Y\}_i$ - target value for i-th object.
- Ordinary least squares (OLS) method:

$$\sum_{n=1}^N\left(x^T\beta-y_n\right)^2=\sum_{n=1}^N\left(\sum_{d=1}^D\beta_d x_n^d-y_n\right)^2\to\min_\beta$$

Solution

Stationarity condition:

$$2\sum_{n=1}^{N} x_n \left(\sum_{d=1}^{D} \beta_d x_n^d - y_n\right) = \mathbf{0}$$

In matrix form:

$$2X^T(X\beta - Y) = \mathbf{0}$$

so

$$\widehat{\beta} = (X^T X)^{-1} X^T Y$$

This is the global minimum, because the optimized criteria is convex.

Linearly dependent features

- Solution $\widehat{\beta}=(X^TX)^{-1}X^TY$ exists when X^TX is non-degenerate
- Problem occurs when one of the features is a linear combination of the other
    - because of the property $\forall X: \; rank(X)=rank(X^TX)$
    - example: constant unity feature c and one-hot-encoding $e_1, e_2, ...e_K$, because $\sum_k e_k \equiv c$
    - interpretation: non-identifiability of $\widehat{\beta}$ for linearly dependent features:
        - linear dependence: $\exists \alpha : \; x^T\alpha = 0 \, \forall x$
        - suppose β solves linear regression $y=x^T\beta$
        - then $x^T\beta \equiv x^T\beta + kx^T\alpha \equiv x^T(\beta+k\alpha)$, so $\beta+k\alpha$ is also a solution!

Linearly dependent features

- Problem may be solved by:
  - feature selection
  - dimensionality reduction
  - imposing additional requirements on the solution (regularization)

Analysis of linear regression

Advantages:

- single optimum, which is global (for non-singular matrix)
- analytical solution
- interpretable solution and algorithm

Drawbacks:

- too simple model assumptions (may not be satisfied)
- $X^T X$ should be non-degenerate (and well-conditioned)

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6. Nadaraya-Watson regression

Generalization by nonlinear transformations

Nonlinearity by x in linear regression may be achieved by applying non-linear transformations to the features:

$$x \to [\phi_0(x), \phi_1(x), \phi_2(x), \dots \phi_M(x)]$$

$$f(x) = \phi(x)^T \beta = \sum_{m=0}^{M} \beta_m \phi_m(x)$$

The model remains to be linear in β, so all advantages of linear regression remain.

Typical transformations

$\phi_k(x)$	**comments**
$x^i \in [a, b]$	binarization of feature
$x^i x^j$	interaction of features
$\exp\left\{-\gamma \left\Vert x - \tilde{x} \right\Vert^2\right\}$	closeness to reference point $\tilde{x}$
$\ln x_k$	the alignment of the distribution with heavy tails
$F^{-1}(x_k)$	conversion of atypical continious distribution to uniform[1]

[1] why?

Non-linear regression

- Alternatively we can model $\mathcal{X} \to \mathcal{Y}$ with arbitrary non-linear function $\widehat{y} = f(x|\theta)$

$$L(\theta|X, Y) = \sum_{n=1}^{N} (f(x_n|\theta) - y_n)^2$$

$$\widehat{\theta} = \arg\min_{\theta} L(\theta|X, Y)$$

- No analytical solution for $\widehat{\theta}$ will exist in general
  - need numeric optimization methods.

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Regularization

- Insert additional requirement for regularizer $R(\beta)$ to be small:

$$\sum_{n=1}^{N}\left(x_n^T\beta - y_n\right)^2 + \lambda R(\beta) \to \min_{\beta}$$

- $\lambda > 0$ - hyperparameter.
- $R(\beta)$ penalizes complexity of models.

$$\begin{array}{ll} R(\beta) = \|\beta\|_1 & \text{Lasso regression} \\ R(\beta) = \|\beta\|_2^2 & \text{Ridge regression} \end{array}$$

- Not only *accuracy* matters for the solution but also *model simplicity*!
- λ controls complexity of the model:

Regularization

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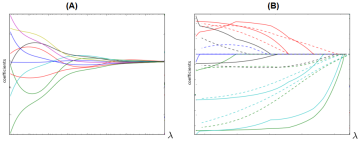
- Not only *accuracy* matters for the solution but also *model simplicity*!
- λ controls complexity of the model:$\uparrow\lambda\Leftrightarrow$ complexity$\downarrow$.

Comments

- Dependency of β from λ for ridge (A) and LASSO (B):



- LASSO can be used for automatic feature selection.
- λ is usually found using cross-validation on exponential grid, e.g. $[10^{-6}, 10^{-5}, ...10^{5}, 10^{6}]$.
- It's always recommended to use regularization because
  - it gives smooth control over model complexity.
  - reduces ambiguity for multiple solutions case.

Ridge regression solution

Ridge regression criterion

$$\sum_{n=1}^{N}\left(x_n^T\beta-y_n\right)^2+\lambda\beta^T\beta\to\min_{\beta}$$

Stationarity condition can be written as:

$$2\sum_{n=1}^{N}x_n\left(x_n^T\beta-y_n\right)+2\lambda\beta=0$$

$$2X^T(X\beta-Y)+\lambda\beta=0$$

$$\left(X^TX+\lambda I\right)\beta=X^TY$$

so

$$\widehat{\beta}=(X^TX+\lambda I)^{-1}X^TY$$

Comments

- $X^TX + \lambda I$ is always non-degenerate as a sum of:
    - non-negative definite X^TX
    - positive definite λI
- Intuition:
    - out of all valid solutions select one giving simplest model
- Other regularizations also restrict the set of solutions.

Different account for different features

- Traditional approach regularizes all features uniformly:

$$\sum_{n=1}^{N}\left(x_n^T\beta-y_n\right)^2+\lambda R(\beta)\to\min_w$$

- Suppose we have K groups of features with indices:

$$I_1, I_2, ...I_K$$

- We may control the impact of each group on the model by:

$$\sum_{n=1}^{N}\left(x_n^T\beta-y_n\right)^2+\lambda_1 R(\{\beta_i|i\in I_1\})+...+\lambda_K R(\{\beta_i|i\in I_K\})\to\min_w$$

- $\lambda_1, \lambda_2, ...\lambda_K$ can be set using cross-validation
- In practice use common regularizer but with different feature scaling.

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Idea

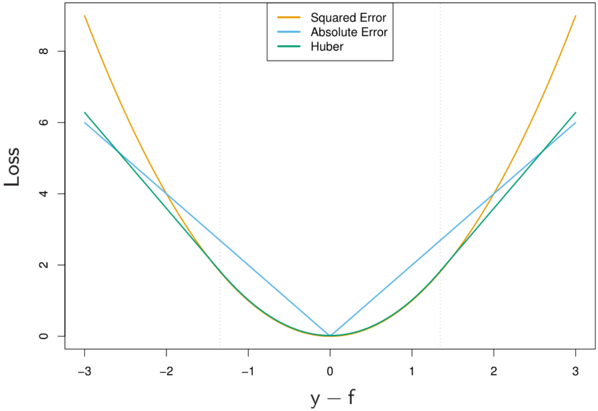
- Generalize quadratic to arbitrary loss:

$$\sum_{n=1}^{N}\left(x^{T}\beta-y_{n}\right)^{2}\to\min_{\beta}\qquad\Longrightarrow\qquad\sum_{n=1}^{N}\mathcal{L}(x_{n}^{T}\beta-y_{n})\to\min_{\beta}$$

LOSS	**NAME**	**PROPERTIES**
$\mathcal{L}(\varepsilon)=\varepsilon^2$	quadratic	differentiable
$\mathcal{L}(\varepsilon)=\lvert\varepsilon\rvert$	absolute	robust
$\mathcal{L}(\varepsilon)=\begin{cases}\frac{1}{2}\varepsilon^2, & \lvert\varepsilon\rvert\le\delta\\ \delta\left(\lvert\varepsilon\rvert-\frac{1}{2}\delta\right) & \lvert\varepsilon\rvert>\delta\end{cases}$	Huber	differentiable, robust

- Robust means solution is robust to outliers in the training set.

Non-quadratic loss functions[2][3]



[2] What is the value of constant prediction, minimizing sum of squared errors?

[3] What is the value of constant prediction, minimizing sum of absolute errors?

Loss function matters

- For $y_1, ...y_N \in \mathbb{R}$ constant minimizers $\widehat{\mu}$:

$$\arg\min_{\mu} \sum_{n=1}^{N} (y_n - \mu)^2 =$$

$$\arg\min_{\mu} \sum_{n=1}^{N} |y_n - \mu| =$$

Loss function matters

- For $y_1, ...y_N \in \mathbb{R}$ constant minimizers $\widehat{\mu}$:

$$\arg\min_{\mu} \sum_{n=1}^{N} (y_n - \mu)^2 = \frac{1}{N} \sum_{n=1}^{N} y_n$$

$$\arg\min_{\mu} \sum_{n=1}^{N} |y_n - \mu| = \text{median}\{y_1, ...y_N\}$$

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- For $x, y \sim P(x, y)$ and functional minimizers $f(x)$:

$$\arg\min_{f(x)} \mathbb{E}\left\{ (f(x) - y)^2 \middle| x \right\} =$$

$$\arg\min_{f(x)} \mathbb{E}\{ |f(x) - y| \, | \, x\} =$$

Loss function matters

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- For $x, y \sim P(x, y)$ and functional minimizers $f(x)$:

$$\arg\min_{f(x)} \mathbb{E}\left\{ (f(x) - y)^2 \middle| x \right\} = \mathbb{E}[y|x]$$

$$\arg\min_{f(x)} \mathbb{E}\left\{ |f(x) - y| \,|\, x \right\} = \text{median}[y|x]$$

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Weighted account for observations[4]

- Weighted account for observations

$$\sum_{n=1}^{N} w_n(x_n^T\beta - y_n)^2$$

- Weights may be:
    - increased for incorrectly predicted objects
        - algorithm becomes more oriented on error correction
    - decreased for incorrectly predicted objects
        - they may be considered outliers that break our model

[4] Derive solution for weighted regression.

Robust regression

- Initialize $w_1 = ... = w_N = 1/N$
- Repeat:
  - estimate regression $\widehat{y}(x)$ using observations (x_i, y_i) with weights w_i.
  - for each $i = 1, 2, ...N$:
    - re-estimate $\varepsilon_i = \widehat{y}(x_i) - y_i$
    - recalculate $w_i = K\left(|\varepsilon_i|\right)$
  - normalize weights $w_i = \frac{w_i}{\sum_{n=1}^{N} w_n}$

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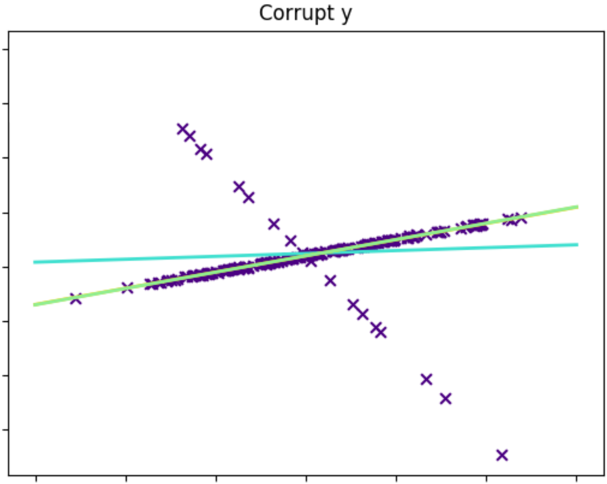
Comments: $K(\cdot)$ is some *decreasing* function, repetition may be

- predefined number of times
- until convergence of model parameters.

Example



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Minimum squared error estimate

For training sample $(x_1, y_1), \dots (x_N, y_N)$ consider finding constant $\widehat{y} \in \mathbb{R}$

$$L(\alpha) = \sum_{i=1}^{N} (\widehat{y} - y_i)^2 \to \min_{\widehat{y} \in \mathbb{R}}$$

$$\frac{\partial L}{\partial \alpha} = 2 \sum_{i=1}^{N} (\widehat{y} - y_i) = 0, \text{ so } \widehat{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

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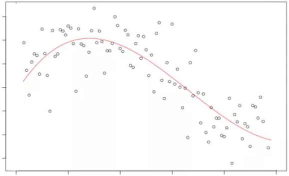
We need to model general curve $y(x)$:



Minimum squared error estimate

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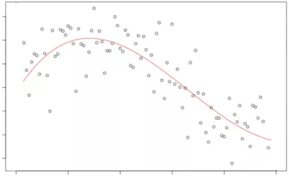
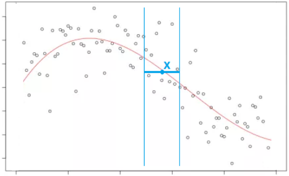


Nadaraya-Watson regression - localized averaging approach.



Nadaraya-Watson regression

- Equivalent names: local constant regression, kernel regression
- For each x assume $\widehat{y}(x) = \alpha = \alpha(x)$, $\alpha \in \mathbb{R}$.

$$Q(\alpha, X_{training}) = \sum_{i=1}^{N} w_i(x)(\alpha - y_i)^2 \to \min_{\alpha \in \mathbb{R}}$$

- Weights depend on the proximity of training objects to the predicted object:

$$w_i(x) = K\left(\frac{\rho(x, x_i)}{h}\right)$$

- $K(u)$ - some decreasing function, called kernel.
- $h(x)$ - some ≥ 0 function called bandwidth.
  - Intuition: "window width", consider $h(x) = h$, $K(u) = \mathbb{I}[u \leq 1]$.

Parameters

- Typically used $K(u)$[5]:

$$\begin{aligned} K_G(u) &= e^{-\frac{1}{2}u^2} \text{ -- Gaussian kernel} \\ K_P(u) &= (1-u^2)^2\mathbb{I}[|u|<1] \text{ -- quartic kernel} \end{aligned}$$

- Typically used $h(x)$:
  - $h(x) = const$
  - $h(x) = \rho(x, x_{i_K})$, where x_{i_K} - K-th nearest neighbour.
    - better for unequal distribution of objects

[5] Compare them in terms of required computation.

Solution

$$Q(\alpha, X_{training}) = \sum_{i=1}^{N} w_i(x)(\alpha - y_i)^2 \to \min_{\alpha \in \mathbb{R}}$$

$$w_i(x) = K\left(\frac{\rho(x, x_i)}{h(x)}\right)$$

- From stationarity condition $\frac{\partial Q}{\partial \alpha} = 0$ obtain optimal $\widehat{\alpha}(x)$:

$$f(x, \alpha) = \widehat{\alpha}(x) = \frac{\sum_{i=1}^{N} y_i w_i(x)}{\sum_{i=1}^{N} w_i(x)} = \frac{\sum_{i=1}^{N} y_i K\left(\frac{\rho(x,x_i)}{h(x)}\right)}{\sum_{i=1}^{N} K\left(\frac{\rho(x,x_i)}{h(x)}\right)}$$

Comments

- Under general regularity conditions $g(x,\alpha) \xrightarrow{P} E[y|x]$
- The specific form of the kernel function does not affect the accuracy much.
    - but may affect efficiency
- Compared to K-NN: may use all objects, bandwidth controls smoothness.
    - under what selection of $K(u)$ and $h(x)$ it reduces to basic K-NN?

Comments

Insead of optimizing locally with constant α

$$Q(\alpha, X_{training}) = \sum_{i=1}^{N} w_i(x)(\alpha - y_i)^2 \to \min_{\alpha \in \mathbb{R}}$$

we could have optimized local linear regression

$$Q(\alpha, X_{training}) = \sum_{i=1}^{N} w_i(x)(x^T\beta - y_i)^2 \to \min_{\alpha \in \mathbb{R}}$$

This better handles approximation on the edges of domain and local extrema.

Summary

- Linear regression gives interpretable analytic solution.
- Non-linear dependencies can be modelled by adding non-linear features.
- When features are correlated, it fails.
- Regularized versions are always preferrable:
    - work in case of correlated features
    - are more robust in close to correlation case
    - λ gives a convenient way to control model complexity
- Robust regression is robust to outliers.
    - we may also use robust loss-functions instead of MSE.