IEMS 304 Lecture 5: Non-linear and Non-parametric Regression

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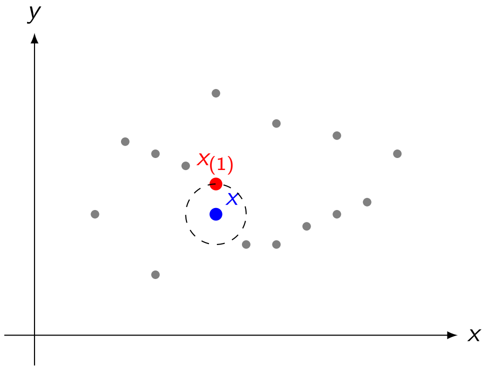
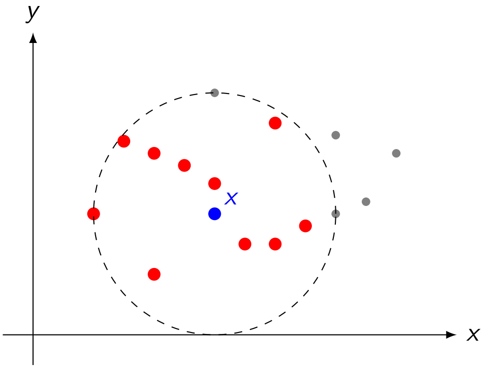
k-NN Regression ($k = 1$)

$$\widehat{f}(x) = y_{(1)}$$



k-NN Regression ($k = 10$)

$$\widehat{f}(x) = \frac{1}{10} \sum_{i=1}^{10} y_{(i)}$$



Non-parametric Statistics

"A precise and universally acceptable definition of the term 'nonparametric' is not presently available. The viewpoint adopted in this handbook is that a statistical procedure is of a nonparametric type if it has properties which are satisfied to a reasonable approximation when some assumptions that are at least of a moderately general nature hold."

– The Handbook of Nonparametric Statistics

Bias and Variance Trade-off

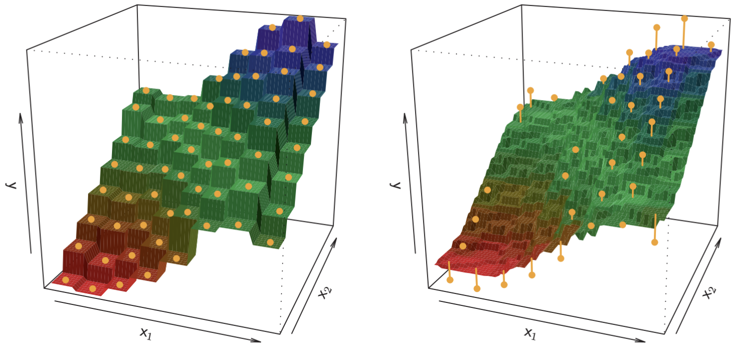
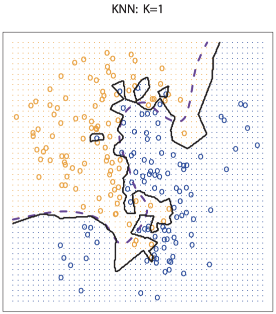
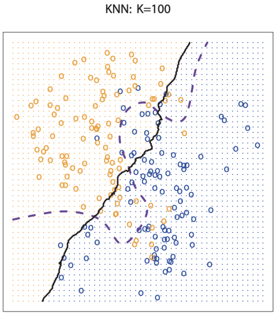
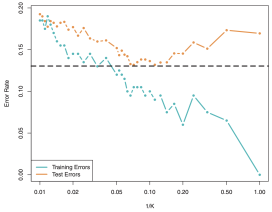


FIGURE 3.16. *Plots of* $\hat{f}(X)$ *using KNN regression on a two-dimensional data set with* 64 *observations (orange dots).* Left: $K = 1$ *results in a rough step function fit.* Right: $K = 9$ *produces a much smoother fit.*

Bias and Variance Trade-off

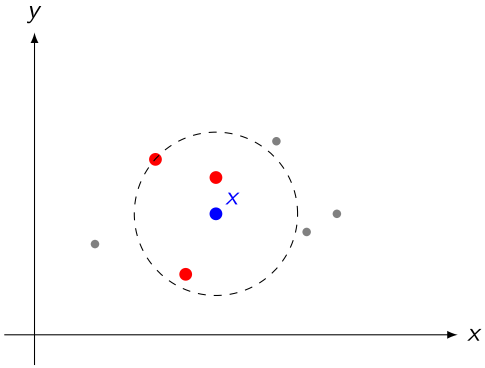






k-NN Regression with Limited Data (k=3)

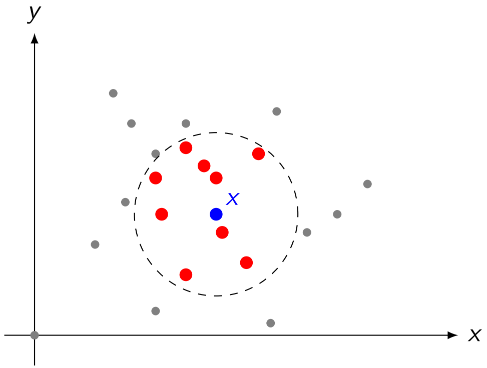
$$\widehat{f}(x) = \frac{1}{3} \sum_{i=1}^{3} y_{(i)}$$



k-NN Regression with More Data

Use the same size of neighborhood, now we have 10 data in the circle

- ❒ How is bais changing? How is variance changing?
- ❒ How should we do bias-variance trade-off?



k-NN Regression with More Data

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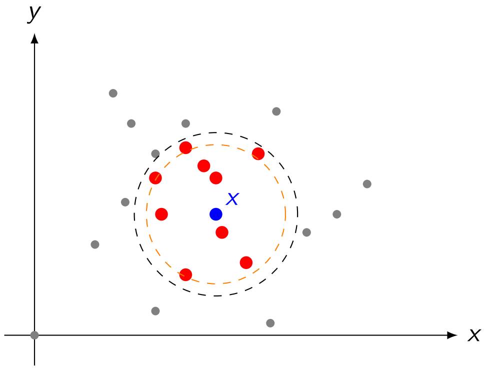
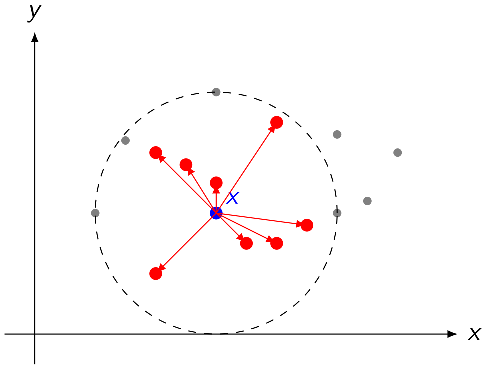
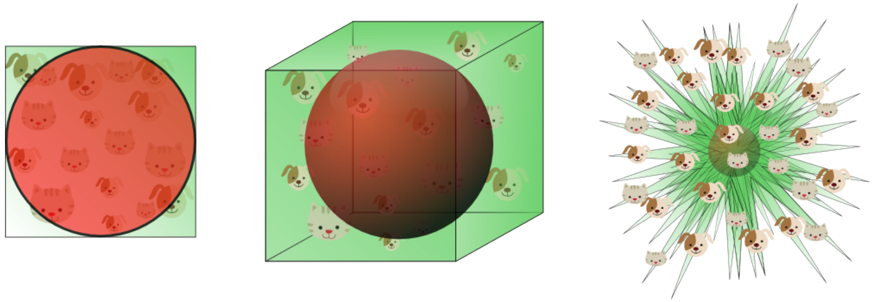


Local Kernel Smoothing: Nadaraya-Watson Estimator

$$\widehat{f}(x) = \frac{\sum_{i=1}^{n} K_h(x - x_i)\, y_i}{\sum_{i=1}^{n} K_h(x - x_i)}$$



Curse of Dimensionality



Nonlinear Regression Models

Nonlinear Regression Model

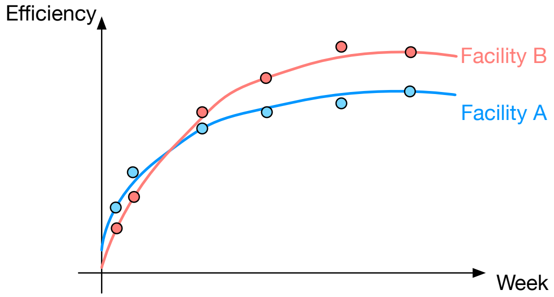
A general form of nonlinear regression model is $Y_i = g(\mathrm{x}_i; \boldsymbol{\beta}) + \epsilon_i$, where

- ❒ Y_i: response for observation i;
- ❒ x_i: vector of predictors for observation i;
- ❒ $\boldsymbol{\beta}$: vector of model parameters;
- ❒ $g(\mathrm{x}_i; \boldsymbol{\beta})$: some parametric nonlinear function;
- ❒ ϵ_i: zero-mean random error for observation i.

We will see shortly that if the random errors are Gaussian and independent of x, the MLE of β is just nonlinear least squares.

Example of Manufacturing Learning Curve

- Two facilities operate with (different) efficiency as a function of time.
- We denote Y as the relative efficiency of operation. The predictor variables are
  - $x_1 = \begin{cases} 1, & \text{facility B (modern)} \\ 0, & \text{facility A (old)} \end{cases}$;
  - $x_2 =$ number of weeks.



Questions and Discussions

- For facility A, and the data looked like in the previous slide, how would you model it?
- Facilities A and B have different asymptotic efficiencies, how would you modify the model?
- If facilities A and B have different learning rates, how would you modify the model?
- If the objective was to determine if the two facilities have different asymptotic efficiencies, how could you do this?

Hint: Play with the model $Y = \beta_0 + \beta_3 \exp(\beta_2 x_2) + \epsilon$.

MLE for General Nonlinear Regression Model

Nonlinear model $Y_i = \underbrace{g(\mathrm{x}_i; \boldsymbol{\beta})}_{:=\mu_i} + \epsilon_i$ with $\epsilon_i \sim \mathrm{N}(0, \sigma^2)$.

Now we view x_i as deterministic, not random.

- Accordingly, the nonlinear model becomes $Y_i = \mu_i + \epsilon_i$.
- Marginal pdf of Y_i is $f(y_i; \boldsymbol{\beta}, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mu_i)^2\right)$.

What is the Max-likelihood Estimator?

Maximizing Likelihood Function

Joint pdf (a.k.a. the likelihood function) of $Y_1, \ldots, Y_n$ is

$$f(\mathrm{y}; \boldsymbol{\beta}, \sigma) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mu_i)^2\right).$$

We want to $\max_{\boldsymbol{\beta},\sigma} f(\mathrm{y}; \boldsymbol{\beta}, \sigma) = \max_{\boldsymbol{\beta},\sigma} \frac{1}{\sigma^n} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mu_i)^2\right)$.

Some inspection suggests that for $\boldsymbol{\beta}$, it suffices to

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^{n}(y_i - \mu_i)^2 = \min_{\boldsymbol{\beta}} \sum_{i=1}^{n}(y_i - \mu_i)^2.$$

log-likelihood

That is, the MLE of $\boldsymbol{\beta}$ for the general nonlinear regression model with i.i.d. Gaussian errors (that are independent of x) is "nonlinear least squares".

How to compute β? Optimization!

Summary of Steps in General MLE

- ❒ Write out the form of the statistical model that you are using to represent the data.
- ❒ Find the marginal distribution of each individual observation Y_i (for regression problems the x_i's are not treated as random, so you only need to find the marginal distribution of the Y_i's given the x_i's).
- ❒ From the marginal distributions in step (2), find the joint distribution $f(\mathrm{Y}; \boldsymbol{\theta})$ of the entire set of data Y. Here $\boldsymbol{\theta}$ denotes all the parameters.

If tractable, find an analytical expression for the $\boldsymbol{\theta}$ that maximizes the likelihood $f(\mathrm{Y}; \boldsymbol{\theta})$. Otherwise, use numerical optimization software to minimize $-\log f(\mathrm{Y}; \boldsymbol{\theta})$.

R for Nonlinear Regression

- R has several built-in commands for nonlinear regression such as nlm and nls (a little buggier than nlm).
- For the manufacturing learning curve example, we read data in `MLC.csv`.
- The following code snippet is for nonlinear regression on `MLC.csv`.

```
MLC<-read.table("MLC.csv",sep=",",header=TRUE)
x1<-MLC$Location;x2<-MLC$Week;y<-MLC$Efficiency
fn <- function(p) {yhat<-p[1]+p[2]*x1+p[4]*exp(p[3]*x2); sum((y-yhat)^2)}
out<-nlm(fn,p=c(1,0,-.5,-.1),hessian=TRUE)
theta<-out$estimate  #parameter estimates
```

Example: Gaussian Distribution with Learned Variance

The likelihood function of a Gaussian distribution is given by:

$$P(y_i \mid \mu(x_i), \sigma(x_i)^2) = \frac{1}{\sqrt{2\pi\,\sigma(x_i)^2}} \exp\left(-\frac{(y_i - \mu(x_i))^2}{2\,\sigma(x_i)^2}\right)$$

$$\begin{aligned}
\ell(\mu, \sigma^2) &= \sum_{i=1}^{n} \log P(y_i | \mu(x_i), \sigma(x_i)^2) \\
&= \sum_{i=1}^{n} \left(-\frac{1}{2}\log(2\pi) - \frac{1}{2}\log(\sigma(x_i)^2) - \frac{(y_i - \mu(x_i))^2}{2\sigma(x_i)^2} \right) \\
&= -\frac{n}{2}\ln(2\pi(x_i)) - \underbrace{\frac{n}{2}\ln(\sigma(x_i)^2)}_{\text{sparse regularization}} - \underbrace{\sum_{i=1}^{n} \frac{(y_i - \mu(x_i))^2}{2\sigma(x_i)^2}}_{\text{weighted } \ell_2 \text{ loss}}
\end{aligned}$$

Another Example: Weibull Distribution

The likelihood function of a Weibull distribution is given by:

$$p_k(x|\lambda) = \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k}$$

, where $1 > k > 0$ is the shape parameter and $\lambda > 0$ is the scale parameter.

$$\log p_k(y|\lambda(x)) = -(y/\lambda(x))^k - k\log\lambda(x) + \underbrace{\log(ky^{k-1})}_{\text{not dependent on the prediction } \lambda(x)}$$

Fact. $f(y, \lambda)$ attains its minimum at $\lambda = y$.

Non-parametric Statistical Inference

Statistical Uncertainty in Supervised Learning

- With nonlinear regression models, the formulae for assessing statistical uncertainty in linear regression (e.g., F-tests and t-tests for significance of predictors, SEs and CIs for parameters, PIs and CIs for new observations, etc.) do not apply directly.
  - Question: Why might we want to calculate SEs, CIs/PIs, do hypothesis tests, etc?
- For some nonlinear models, we can use approximate **asymptotic analytical results** valid for sufficiently large sample size n to assess statistical uncertainty.
- Fortunately, we have alternative **computational approaches** that apply to any nonlinear model:
  - **Cross-validation** for deciding which models are the best.
  - **Bootstrap resampling** (or **bootstrapping** for short) for SEs and CIs on the parameters and CIs and PIs on new observations.

Overview of Bootstrapping

Objective: Estimate the sampling distribution of $\widehat{\boldsymbol{\theta}}$ and quantities like $\mathrm{SE}(\widehat{\boldsymbol{\theta}})$ that are derived from it.

❒ You are given a sample of data of size *n* observations.

❒ You have estimated some parameter(s) $\boldsymbol{\theta}$ (call it $\widehat{\boldsymbol{\theta}}$).

Problem: Hypothetically, if we knew the form of the population distribution, we could consider using simulation to draw many random samples (each of size *n*) from the population and calculate a different $\widehat{\boldsymbol{\theta}}$ for each sample. We could construct a histogram of all the $\widehat{\boldsymbol{\theta}}$'s and take their sample standard deviation to be an estimate of $\mathrm{SE}(\widehat{\boldsymbol{\theta}})$. But what if we do not know the form of the population distribution?

Illustration of Sampling from Known Distribution

AIM. estimate the mean of a Gaussian distribution and want to known the SE of the estimate.

- ❒ Generate say 10,000 samples, each of size $n = 20$, from an $\mathrm{N}(5.3, 0.4^2)$ distribution.
- ❒ Calculate the averages $\{\bar{y}_{\text{sim}}^{(j)} : j = 1, \ldots, 10000\}$ for the 10000 replicates.
- ❒ Take

$$\mathrm{SE}(\bar{y}) \approx \sqrt{\frac{1}{10000 - 1} \sum_{j=1}^{10000} (\bar{y}_{\text{sim}}^{(j)} - \bar{y}_{\text{sim}})^2},$$

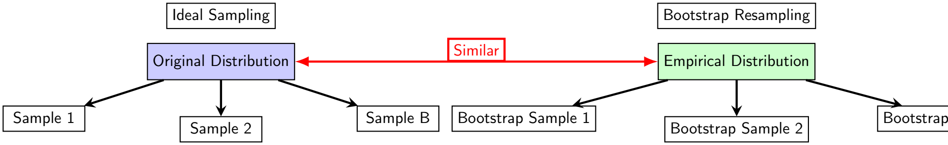
where $\bar{y}_{\text{sim}}$ is the average of $\bar{y}_{\text{sim}}^{(j)}$.

Idea: Bootstrap Sampling

However, Step:

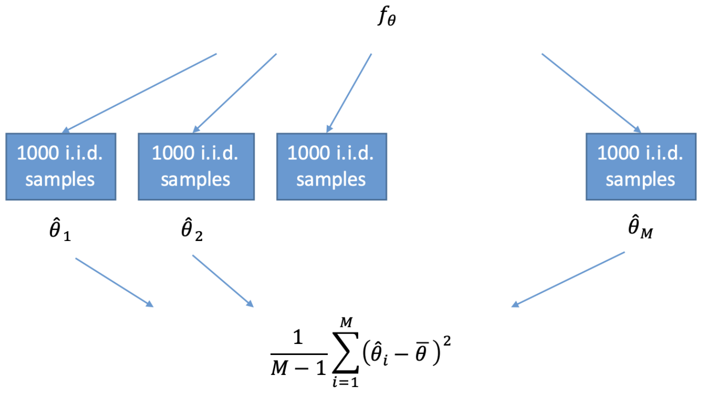
Generate say 10,000 samples, each of size $n = 20$, from $\underbrace{\mathrm{N}(5.3, 0.4^2)}_{\text{population}}$ is impossible!

Idea. Bootstrap Sampling



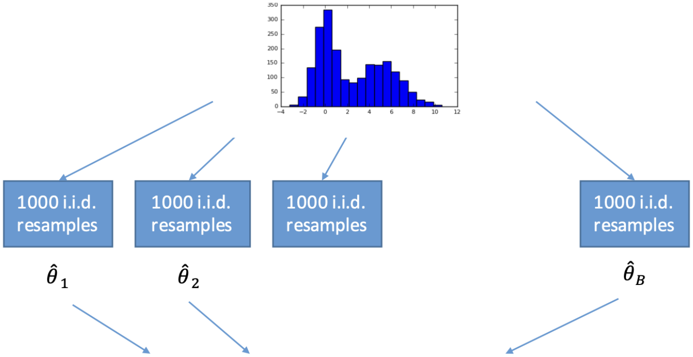
Idea:

If we know f_θ, we can generate new samples to recompute the statistic, and take the sample variance of these estimators



Realisitic

Idea: use the observed samples $z_1, \ldots, z_n$ to generate n "new" samples, as if they come from



$$\frac{1}{B-1}\sum_{i=1}^{B}\left(\hat{\theta}_i - \bar{\theta}\right)^2$$

Bootstrapping Overview Cont'd

- The **bootstrap sampling approach**: Draw a "bootstrap" sample as a random sample of the same size n from the original sample of n observations (with replacement), and calculate a $\widehat{\boldsymbol{\theta}}$ for the bootstrap sample.
- Repeat a large number of times, each time drawing another bootstrap sample (of size n) and calculating another $\widehat{\boldsymbol{\theta}}$ for that sample.
- Then construct a histogram of all the $\widehat{\boldsymbol{\theta}}$'s, take their sample standard deviation to be an estimate of $\mathrm{SE}(\widehat{\boldsymbol{\theta}})$, etc.

Why this works: Consider making a pretend population that consists of your original sample of n observations, copied over and over, an infinite number of times. Each bootstrap sample is equivalent to drawing a random sample of size n from this infinite pretend population.

Illustration of Bootstrapping

AIM. estimate the mean of an unknown distribution and want to known the SE of the estimate.

- Generate say 10,000 samples, each of size $n = 20$, from the given **observed data** (with replacement).
- Calculate the averages $\{\bar{y}^{(b)} : b = 1, \ldots, 10000\}$ for the 10000 replicates. (We think of $\bar{y}^{(b)}$ just as the estimator $\widehat{\theta}$.)
- Take

$$\mathrm{SE}(\bar{y}) \approx \sqrt{\frac{1}{10000 - 1} \sum_{j=1}^{10000} (\bar{y}^{(b)} - \bar{y})^2},$$

where $\bar{y}$ is the average of $\bar{y}^{(b)}$.

Bootstrapping in Nonlinear Regression

- We have a sample of n observations $\{(y_i, \mathrm{x}_i)\}_{i=1}^{n}$ of a response variable and a set of predictor variables.
- We fit a nonlinear regression model to the data to estimate a set of parameters $\boldsymbol{\theta}$.
- Let θ denote one of the parameters of interest and $\widehat{\theta}$ its estimate.

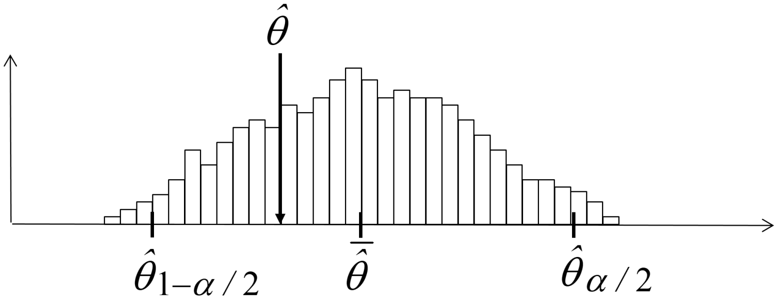
Objective: Estimate the sampling distribution of $\widehat{\theta}$, its standard error, a confidence interval for θ, etc.

Steps of the Bootstrap Procedure

- ❒ Generate a "bootstrap" sample (with replacement) of n observations from $\{(y_i, \mathrm{x}_i)\}_{i=1}^n$. Denote the bootstrap sample by
$$\{(y_i^{(b)}, \mathrm{x}_i^{(b)})\}_{i=1}^n.$$
- ❒ Fit the same type of regression model (with the same set of parameters $\boldsymbol{\theta}$ and parameter θ of special interest) to the bootstrapped sample. Denote the estimates for the bootstrapped sample by $\widehat{\boldsymbol{\theta}}^{(b)}$ and $\widehat{\theta}^{(b)}$.
- ❒ Pick a large number B (e.g., $B = 10,000$), and repeat Steps (1) and (2) a total of B times, which produces
$$\{\widehat{\theta}^{(b)}\}_{b=1}^B.$$

Steps of the Bootstrap Procedure Cont'd

- Construct a histogram of $\{\widehat{\theta}^{(b)}\}_{b=1}^{B}$ and calculate
  - $\overline{\widehat{\theta}} = \frac{1}{B}\sum_{b=1}^{B}\widehat{\theta}^{(b)}$: average of all bootstrapped estimates.
  - $\mathrm{SE}(\widehat{\theta}) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}(\widehat{\theta}^{(b)} - \overline{\widehat{\theta}})}$: standard error of $\widehat{\theta}$.
  - $\widehat{\theta}_{\alpha/2}$: upper $\alpha/2$ quantile.
  - $\widehat{\theta}_{1-\alpha/2}$: lower $\alpha/2$ quantile.


$\hat{\theta}$
$\hat{\theta}_{1-\alpha/2}$
$\overline{\hat{\theta}}$
$\hat{\theta}_{\alpha/2}$

Some Output of Bootstrap

- A crude $1-\alpha$ confidence interval for θ is
$$\widehat{\theta} - z_{\alpha/2} \cdot \mathrm{SE}(\widehat{\theta}) \le \theta \le \widehat{\theta} + z_{\alpha/2} \cdot \mathrm{SE}(\widehat{\theta}).$$
- A better $1-\alpha$ confidence interval for θ is
$$\widehat{\theta} - (\widehat{\theta}_{\alpha/2} - \widehat{\theta}) \le \theta \le \widehat{\theta} + (\widehat{\theta} - \widehat{\theta}_{1-\alpha/2}).$$

Conformal Prediction

Conformal Prediction

AIM.

❒ Finite-sample coverage guarantees without distributional assumptions

❒ Converting a point prediction algorithm into a prediction set

- **Input:** i.i.d. data pairs (X_i, Y_i) for $i = 1, \ldots, n$
- **Objective:** Construct a prediction band $\widehat{C}_n(x)$ such that

$$P\big(Y_{n+1} \in \widehat{C}_n(X_{n+1})\big) \geq 1 - \alpha$$

Note: Trivial solutions (Why?) exist, but the goal is to develop nontrivial, adaptive methods

Key Idea: Using Ranks and Quantiles

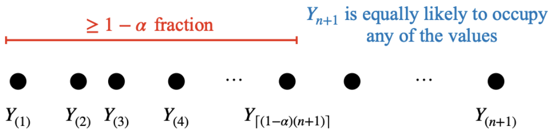
Observation. the rank of Y_{n+1} is uniformly distributed over the values $1, 2, \ldots, n+1$. This means that

$$P\Big(Y_{n+1} \text{ is among the } \lceil(1-\alpha)(n+1)\rceil \text{ smallest of } Y_1, \ldots, Y_n\Big) = 1-\alpha,$$

which is in turn equivalent to[1]

$$P\Big(Y_{n+1} \text{ is among the } (1-\alpha)(n+1) \text{ smallest of } Y_1, \ldots, Y_n\Big) \geq 1-\alpha.$$

Accordingly, by defining $q_n =$ the $\lceil(1-\alpha)(n+1)\rceil$-th smallest of $Y_1, \ldots, Y_n$, we have precisely achieved the desired property. via $Y_{n+1} \leq$ the $\lceil(1-\alpha)(n+1)\rceil$-th order statistic of $Y_1, \ldots, Y_n$.


$\geq 1-\alpha$ fraction
Y_{n+1} is equally likely to occupy any of the values
$Y_{(1)}$
$Y_{(2)}$
$Y_{(3)}$
$Y_{(4)}$
$\cdots$
$Y_{\lceil(1-\alpha)(n+1)\rceil}$
$\cdots$
$Y_{(n+1)}$

Full Conformal Prediction

We havei.i.d. pairs $\{(X_t, Y_t)\}_{t=1}^{n}$, where $X_t \in \mathcal{X}$ and $Y_t \in \mathcal{Y}$. We want to construct a prediction set for Y_{n+1} given X_{n+1}. Let $\widehat{f}_n$ be any regression predictor trained on

$$(X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n).$$

Our goal is to achieve $(1-\alpha)$ coverage, i.e.,

$$P\big(Y_{n+1} \in C_n(X_{n+1})\big) \;\geq\; 1-\alpha.$$

Why the Naive procedure Fails?

- ❒ Compute the *training residuals* $\widehat{g}_i \;=\; Y_i \;-\; \widehat{f}_n(X_i), \quad i = 1, 2, \dots, n.$
- ❒ Let $\widehat{q}_n$ be an estimate of a suitable quantile of the absolute residuals, for example the $(1-\alpha)$ empirical quantile of

$$\big\{|\widehat{g}_1|, |\widehat{g}_2|, \dots, |\widehat{g}_n|\big\}.$$

- ❒ Define the prediction set for a new point x as

$$C_n(x) \;=\; \Big[\,\widehat{f}_n(x) \;-\; \widehat{q}_n,\;\; \widehat{f}_n(x) \;+\; \widehat{q}_n\Big].$$

Full Conformal Prediction

We havei.i.d. pairs $\{(X_t, Y_t)\}_{t=1}^n$, where $X_t \in \mathcal{X}$ and $Y_t \in \mathcal{Y}$. We want to construct a prediction set for Y_{n+1} given X_{n+1}. Let $\widehat{f}_n$ be any regression predictor trained on

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Our goal is to achieve $(1-\alpha)$ coverage, i.e.,

$$P\big(Y_{n+1} \in C_n(X_{n+1})\big) \;\geq\; 1-\alpha.$$

Full Conformal Prediction

- Compute the *training residuals* $\widehat{g}_i \;=\; Y_i \;-\; \widehat{f}^{-i}{}_n(X_i), \quad i = 1, 2, \dots, n.$

  ($-i$ means delete $i-$th data while training)

- Let $\widehat{q}_n$ be an estimate of a suitable quantile of the absolute residuals, for example the $(1-\alpha)$ empirical quantile of $\big\{|\widehat{g}_1|, |\widehat{g}_2|, \dots, |\widehat{g}_n|\big\}$.
- Define the prediction set for a new point x as

$$C_n(x) \;=\; \Big[\, \widehat{f}_n(x) \;-\; \widehat{q}_n,\;\; \widehat{f}_n(x) \;+\; \widehat{q}_n \Big].$$

Split Conformal Prediction

Full Conformal Prediction is computationally intractable! (**why**?)

Key Idea. Data Split

❒ **Proper Training Set (D_1):** Fit the point predictor $\widehat{f}_{n_1}(x)$

❒ **Calibration Set (D_2):** Compute residuals

$$R_i = |Y_i - \widehat{f}_{n_1}(X_i)|, \quad i \in D_2$$

- Define quantile from calibration residuals:

$$q_{n_2} = \lceil (1-\alpha)(n_2+1) \rceil\text{-th smallest residual}$$

- Prediction set:

$$\widehat{C}_n(x) = \left[\widehat{f}_{n_1}(x) - q_{n_2},\ \widehat{f}_{n_1}(x) + q_{n_2}\right]$$

- Guarantee: Ensures marginal coverage of at least $1-\alpha$

Mathematical Formulation: Regression Case

Nonconformity Score

For a predictive model $\widehat{f}$ and calibration data $\{(x_i, y_i)\}_{i=1}^{n_{\text{cal}}}$, define the nonconformity score as:

$$\alpha_i = \left| y_i - \widehat{f}(x_i) \right|$$

Prediction Interval

Let $\widehat{q}_{1-\alpha}$ be the $(1-\alpha)$-quantile of $\{\alpha_i\}_{i=1}^{n_{\text{cal}}}$. For a new input x_{n+1}, the prediction interval is given by:

$$\{y \in \mathbb{R} : \left| y - \widehat{f}(x_{n+1}) \right| \leq \widehat{q}_{1-\alpha}\}$$

This interval guarantees that the true y falls inside with probability at least $1 - \alpha$.

Mathematical Formulation: Classification Case

Nonconformity Score

For a classification model, a common choice is:

$$\alpha_i = 1 - p(y_i \mid x_i)$$

where $p(y_i \mid x_i)$ is the predicted probability for the true class.

Prediction Set

For a new example x_{n+1}, the prediction set is defined as:

$$\Gamma(x_{n+1}) = \left\{ y \in \mathcal{Y} : \frac{\#\{i : \alpha_i \geq \alpha(y)\} + 1}{n_{\text{cal}} + 1} > \alpha \right\}$$

where $\alpha(y)$ is the nonconformity score computed if y were the true label.

Advantages and Limitations

Advantages

- **Finite-Sample Guarantees:** Ensures valid coverage without asymptotic approximations.
- **Model-Agnostic:** Can be applied on top of any predictive model.

Limitations

- **Computational Cost:** Some methods can be computationally intensive, especially in the transductive setting.
- **Loose Confidence Interval**
- **Assumptions:** Relies on the exchangeability assumption which might not hold in all cases.