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STAT 444/844 Course Notes

Statistical Learning: Function Estimation

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Abstract

These notes are intended as a resource for myself; past, present, or future students of this course, and anyone interested in the material. The goal is to provide an end-to-end resource that covers all material discussed in the course displayed in an organized manner. These notes are my interpretation and transcription of the content covered in lectures. The instructor has not verified or confirmed the accuracy of these notes, and any discrepancies, misunderstandings, typos, etc. as these notes relate to course's content is not the responsibility of the instructor. If you spot any errors or would like to contribute, please contact me directly.

1 January 8, 2019

1.1 What is a function?

Suppose we have some measured **response** variate y and we have one or more **explanatory** variables $x_1, \ldots, x_p$. The response and explanatory ariables are approximately related through an unknown function $\mu(x)$ (to be estimated/learned) where

$$y = \mu(x) + r$$

where r is residual that cannot be explained by $\mu(x)$.
Some other names for response and explanatory variables include:

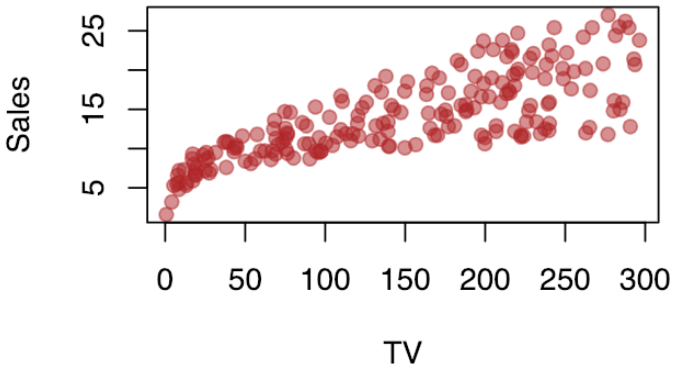
response	explanatory
response	predictor
response	design
output	input
dependent	independent
endogenous	exogenous

1.2 Advertising data example

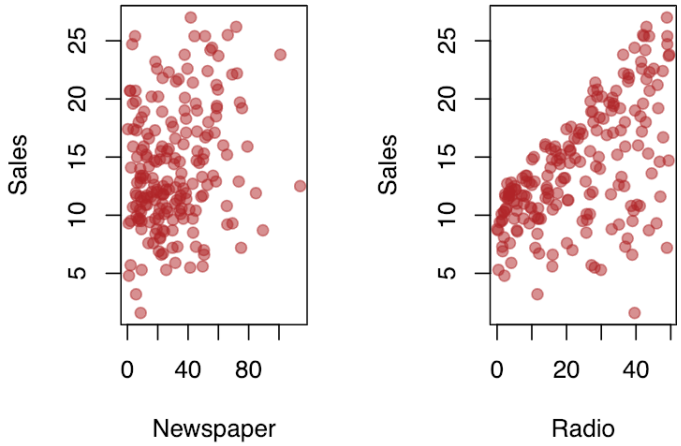
Suppose we want to predict Sales (response) from how much companies spend on TV, Radio, and Newspaper advertising (explanatory).
The dataset is

```
##   X    TV Radio Newspaper Sales
## 1 1 230.1  37.8      69.2  22.1
## 2 2  44.5  39.3      45.1  10.4
## 3 3  17.2  45.9      69.3   9.3
## 4 4 151.5  41.3      58.5  18.5
## 5 5 180.8  10.8      58.4  12.9
## 6 6   8.7  48.9      75.0   7.2
```

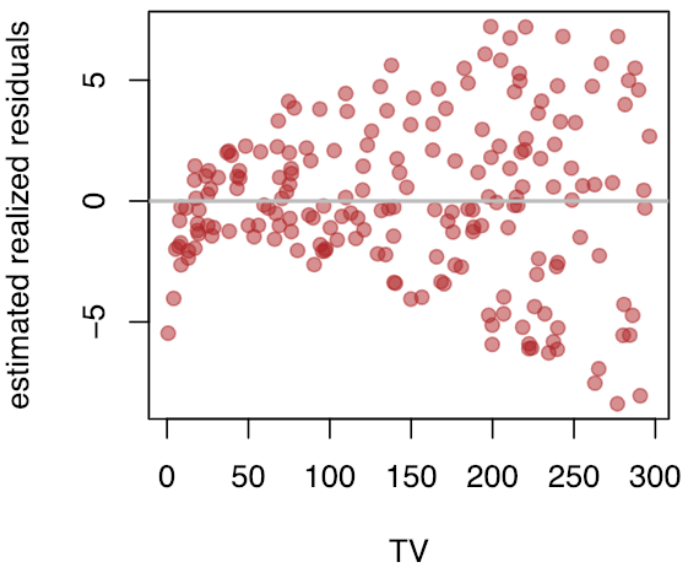
if we plot sales against TV



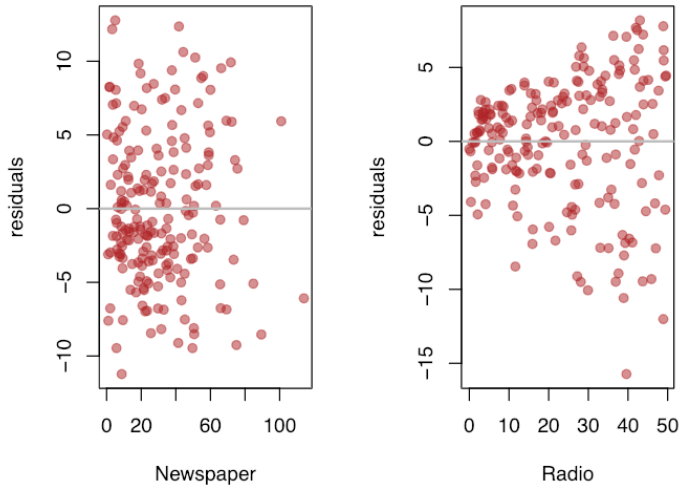
we see there is some positive correlation.
Similarly against Newspaper and Radio



What if we tried a simple linear model where $\hat{\mu}(x_1) = \hat{\alpha} + \hat{\beta}x_1$ where x_1 is the TV advertising? We obtain estimates $\hat{\alpha} = 7.03$ and $\hat{\beta} = 0.05$ which are interpretable. However if we take a look at the residuals



we see that the residuals are not independently distributed accordingly to x_1, which violates our Markov-Gaussian assumptions.
The residuals of the model with Newspaper and Radio are



we observe that we do not observe constant variance across the explanatory variables.
Therefore a linear model does not seem to work (we could of course introduce scaling e.g. log-scaling for the Radio variate or polynomial terms).

1.3 Notation

Some notes on notation:

- Capital letters are matrices or vectors: A, X, Σ
- Lower letters are scalars: a, x, σ

- Arrows on letters are vectors: $\vec{a}, \vec{x}$
- All vectors are column vectors
- The transpose of any matrix A is A^T (ocassionally A')

1.4 Definitions and properties

Quadratic form Suppose $A = (a_{ij})_{n\times n}$ is symmetric i.e. $a_{ij} = a_{ji}\ \forall i, j$. Then

$$\begin{aligned} f &= Y^T A Y \\ &= \sum_i \sum_j a_{ij} y_i y_j \end{aligned}$$

is called a **quadratic form**.

Trace For a matrix, the **trace** is defined as

$$\text{tr}(A_{m\times m}) = \sum_{i=1}^{m} a_{ii}$$

Note that $\text{tr}(BC) = \text{tr}(CB)$.

Rank The **rank** of a matrix denoted $\text{rank}(A)$ is the maximum number of *linearly independent columns* (or rows) of A.

Note that vectors $Y_1, \ldots, Y_n$ are linearly independent iff

$$c_1 Y_1 + \ldots + c_n Y_n = 0$$

implies $c_1 = \ldots = c_n = 0$ (i.e. no non-trivial solution).

Eigenvector and eigenvalue A non-zero vector $\vec{v}_i$ is an **eigenvector** of $A_{m\times m}$ if

$$A\vec{v}_i = \lambda_i \vec{v}_i \qquad i = 1, 2, \ldots, m$$

where λ_i is the corresponding ith **eigenvalue**.

Idempotent A matrix A is **idempotent** if $AA = A$.

Some notable results:

1. If A is idempotent, then all its eigenvalues are either 0 or 1.
2. If A is idempotent, there exists an orthogonal matrix P such that $A = P\Lambda P^T$ where

$$\Lambda = \begin{bmatrix} 1 & \ldots & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 & 0 \\ 0 & \ldots & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ldots & 0 \end{bmatrix}$$

and $\text{tr}(A) = \text{rank}(A) = \text{tr}(\Lambda)$ which is equivalent to the number of eigenvalues being 1.

2 January 10, 2019

2.1 Linear models

A linear model is generally in the form of

$$y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \epsilon_i \qquad i = 1, \ldots, n$$

which holds under the assumptions that

- $E(\epsilon_i) = 0$
- $Var(\epsilon_i) = \sigma^2$ (constant variance)
- $\epsilon_1, \ldots, \epsilon_n$ are independent
- $\epsilon_1, \ldots, \epsilon_n \overset{iid}{\sim} N(0, \sigma^2)$

In matrix form we have

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}_{n\times 1} = \begin{bmatrix} 1 & x_{11} & \ldots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{np} \end{bmatrix}_{n\times(p+1)} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}_{(p+1)\times 1} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}_{n\times 1}$$

or in short matrix form $Y = X\vec{\beta} + \vec{\epsilon}$.
The **Least Squares Estimator (LSE)** of $\vec{\beta}$ minimizing the discrepancy function

$$S(\vec{\beta}) = (Y - X\vec{\beta})^T (Y - X\vec{\beta})$$

has a closed form solution

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

The fitted values are thus

$$\begin{aligned} \hat{Y} = X\hat{\vec{\beta}} &= X(X^T X)^{-1} X^T Y \\ &= HY \end{aligned}$$

where $H = X(X^T X)^{-1} X^T$ (**hat matrix**). Note that H is **idempotent** and **symmetric**.
Geometric interpretation of LSE: $\hat{Y}$ is the projection of Y onto $C(X)$, the column space of X (we can thus see that the fitted errors should be orthogonal to our fitted values in LSE).
The **degrees of freedom** of our model is $n - (p+1)$ where $p+1$ is the number of free parameteres in our model. This is equivalent to $n - \text{tr}(H)$ i.e. $\text{tr}(H) = p + 1$.
Under normality

- $\hat{\vec{\beta}} = MVN(\vec{\beta}, \sigma^2 (X^T X)^{-1})$
- $\hat{\vec{\beta}}$ and $\hat{\sigma}^2$ are independent (Note $\hat{\sigma}^2 = \frac{SSE}{df}$).
- $\frac{(n-p-1)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p-1}$

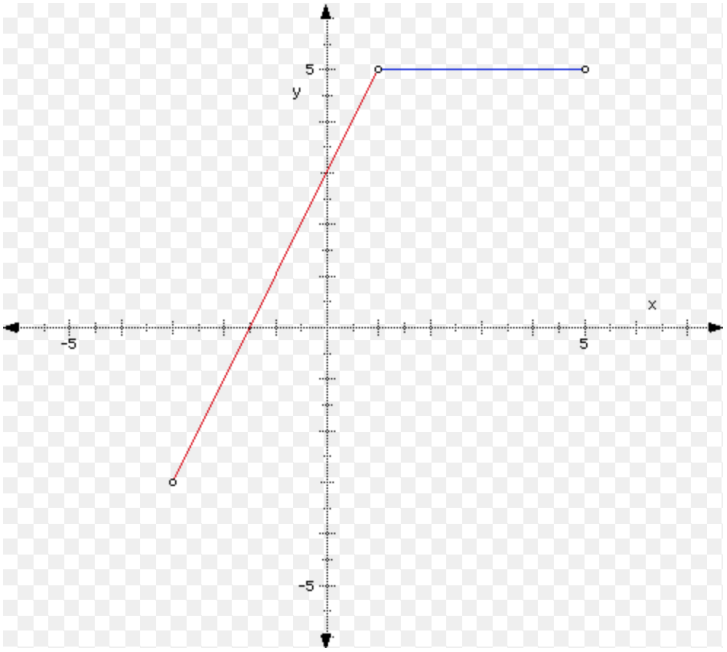
Let $\vec{a}_p = (1, x_1, \ldots, x_p)^T$ (observation $\vec{x}$ extended with intercept term). The $(1-\alpha)$ **prediction interval** at $\vec{a}_p$ is

$$\vec{a}_p^T \hat{\vec{\beta}} \pm t_{n-p-1,\alpha/2} \hat{\sigma} \sqrt{1 + \vec{a}_p^T (X^T X)^{-1} \vec{a}_p}$$

We can also estimate **confidence intervals** as well (drop $1 + \ldots$ term above).

2.2 Piecewise linear

We can specify the following piecewise linear function (with discontinuity at a)



as two linear functions

$$y = \begin{cases} \beta_0 + \beta_1 x & x \leq a \\ \beta_2 + \beta_3 x & x \geq a \end{cases}$$

subject to $\beta_0 + \beta_1 a = \beta_2 + \beta_3 a$.
A more convenient way to express the above

$$y = \beta_0 + \beta_1 x + \beta_2 (x - a) I(x \geq a)$$

where I is the indicator function. Note the above is linear in terms of $\vec{\beta}$ BUT NOT in terms of x. However we can simply construct a new variate $(x-a)I(x \geq a)$ from x.
Note that β_2 is the *change in slope right of* a for samples where $x \geq a$.
Extension to more than one interesting point (knot) is straightforward.

2.3 Piecewise quadratic

Similar to piecewise linear models, we can specify

$$y = \begin{cases} \beta_0 + \beta_1 x + \beta_2 x^2 & x \leq a \\ \beta_3 + \beta_4 x + \beta_5 x^2 & x \geq a \end{cases}$$

subject to $\beta_0 + \beta_1 a + \beta_2 a^2 = \beta_3 + \beta_4 a + \beta_5 a^2$ (continuity) and $\beta_1 + 2\beta_2 a = \beta_4 + 2\beta_5 a$ (differentiable at a). Alternatively we can express this as one linear function

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 (x-a)^2 I(x \geq a)$$

continuity is trivially satisfied. Note the 1st derivative is

$$\frac{dy}{dx} = \beta_1 + \beta_2 x + 2\beta_3 (x-a) I(x \geq a)$$

where the last term is 0 when $x = a$, thus our additional indicator term does not affect the derivative.

Remark 2.1. We choose to omit the $(x-a)I(x \geq a)$ term to ensure y is differentiable at $x = a$.

2.4 Weighted least squares

Sometimes we would like to give more importance to some observations than others.
Instead of minimizing $(Y - X\vec{\beta})^T (Y - X\vec{\beta})$ we can minimize

$$(Y - X\vec{\beta})^T W (Y - X\vec{\beta})$$

where

$$W = \begin{bmatrix} w_1 & 0 & \dots & 0 \\ 0 & w_2 & \dots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \dots & w_n \end{bmatrix}_{n \times n}$$

a diagonal matrix. w_i corresponds to the weight assigned to observation i (a higher w_i the more important that observation is).

Claim. The closed form solution is

$$\hat{\vec{\beta}}_{WLS} = (X^T W X)^{-1} X^T W Y$$

Proof. Note that

$$\begin{aligned} S(\vec{\beta}) &= (Y - X\vec{\beta})^T W (Y - X\vec{\beta}) \\ &= Y^T W Y - Y^T W X \vec{\beta} - \vec{\beta}^T X^T W Y + \vec{\beta}^T X^T W X \vec{\beta} \end{aligned}$$

Note that $Y^T W X \vec{\beta} = (\vec{\beta}^T X^T W Y)^T$ which is a scalar, so $Y^T W X \vec{\beta} = \vec{\beta}^T X^T W Y$ (transposes of scalars are equivalent). thus

$$S(\vec{\beta}) = Y^T W Y - 2 Y^T W X \vec{\beta} + \vec{\beta}^T X^T W X \vec{\beta}$$

where $-2Y^T W X \vec{\beta}$ is the "linear term" and $\vec{\beta}^T X^T W X \vec{\beta}$ is of quadratic form.

Recall that

$$\frac{d\vec{c}^T Y}{dY} = \vec{c}^T$$
$$\frac{dY^T AY}{dY} = 2Y^T A^T$$

so

$$\frac{dS(\vec{\beta})}{d\vec{\beta}} = -2Y^T WX + 2\vec{\beta}^T X^T WX$$
$$\Rightarrow \vec{\beta}^T X^T WX = Y^T WX \qquad \frac{dS(\vec{\beta})}{d\vec{\beta}} = 0$$
$$\Rightarrow (X^T WX)\vec{\beta} = X^T WY \qquad W^T = W$$
$$\Rightarrow \vec{\beta} = (X^T WX)^{-1} X^T WY$$

as claimed. □

Here is an alternative proof:

Proof. Let $Y^* = W^{\frac{1}{2}} Y$ and $X^* = W^{\frac{1}{2}} X$.
Note that minimizing $(Y - X\vec{\beta})^T W(Y - X\vec{\beta})$ is equivalent to minimizing $(Y^* - X^*\vec{\beta})^T(Y^* - X^*\vec{\beta})$ (simply expand out X^* and Y^*).
Thus the LSE of $\vec{\beta}$ with X^*, Y^* is

$$\begin{aligned}\vec{\beta} &= (X^{*^T} X)^{-1} X^{*^T} Y^* \\ &= ((X^T W^{\frac{1}{2}})(W^{\frac{1}{2}} X))^{-1}(X^T W^{\frac{1}{2}})(W^{\frac{1}{2}} Y) \\ &= (X^T WX)^{-1} X^T WY\end{aligned}$$

which is equivalent to our previous derivation. □

3 January 15, 2019

3.1 Weight least squares applications

Example 3.1. We can apply weighted least squares to do **local regression** where we downweight observations farther away from a given observation.

Example 3.2. Suppose that $Var(\epsilon_i) = \sigma_i^2$ (i.e. not all observations are drawn with the same variance). If we want to overweight observations that have lower variance, we can set $w_i = \frac{1}{\sigma_i^2}$ to obtain an **unbiased estimator of** $\vec{\beta}$ with the *smallest variance* (**Best Linear Unbiased Estimator** or **BLUE**).

3.2 Types of errors

We will use the example of 790 *Facebook* posts published by a comestics company to illusrate.
The population being examined is called the **study population** (the 790 posts). The analysis of these posts may be applied to a larger population (whether it's future Facebook posts for this company or Facebook posts for *any* company) which we call the **targt population**.
The difference between the study and target population is called the **study error**.

In a paper by Soros et al., they ended up using a **sample** of only 500 posts for confidentiality reasons.
The difference between the sample and study population is called **sample error**.

4 January 17, 2019

4.1 Notes on terminology and `lm` in R

- When using `lm` the intercept term is included by default. To remove it simply specify `Y ~ X - 1`.
- **Factors** are like categorical variables in R: there are a finite number of categories (called **factor levels**).
- In `lm` almost any function of variates may appear in the formula e.g. `Y ~ X + sin(X)` or `Y ~ X + sin(X * Y)`.

  To specify $Y = X \cdot Z$, we need to use `Y ~ I(X * Z)` or `Y ~ X:Z` *instead of* `X * Z` since `X * Z` represents **interaction** in `lm` and translates to the model $y = \alpha x + \beta z + \gamma xz + r$.
- Some arithmetic operations e.g. $+, -, *, \hat{}$ are interpreted as formula operators rather than arithmetic operators in `lm`. One should wrap them in `I(·)`.

4.2 Notes on model selection

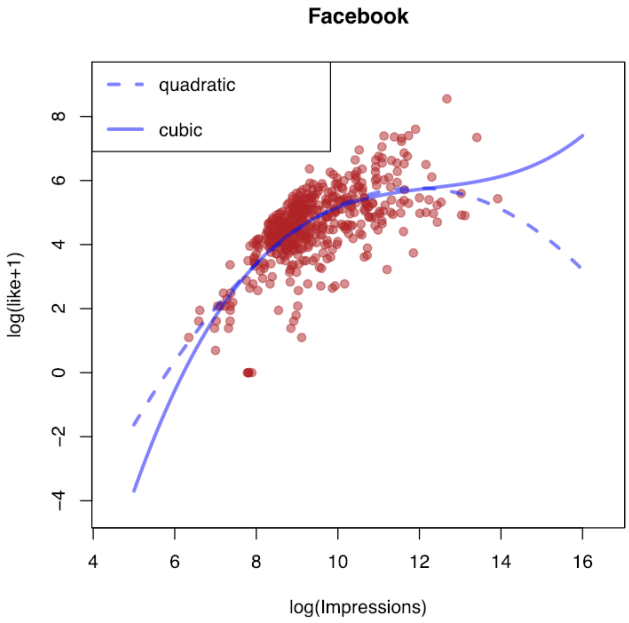


Figure 4.1: Quadratic and cubic polynomial linear models on Facebook data.

In the above figure we see that while both quadratic and cubic models are **global** (predict any value of x) the quadratic model seems to predict likes returning to 0 as impressions approach infinity.
The cubic function on the contrary continues to increase: this makes more sense intuitively, thus examining a model often requires human understanding of the data and problem.

4.3 Geometric interpretation of linear models

A linear model is a linear combination of functions called **generators** e.g.

$$\mu(x) = \beta_1 g_1(x) + \beta_2 g_2(x) + \beta_3 g_3(x) + \beta_4 g_4(x)$$

where $g_1, \ldots, g_4$ could be arbitrary continuous functions of x.
All possible linear combinations of the generators forms a **subspace** (the functions *generate* the subspace). The functions are a **basis** for this subspace. $\mu(x)$ lies in the subspace whose dimension equals to the number of basis functions.
The functions should be *linearly independent* of each other: otherwise the solution to parameters will be ill-defined.

5 January 24, 2019

5.1 Discrepancy function

Let the **discrepancy function** for a fit of parameters $\vec{\beta}$ be denoted

$$S(\vec{\beta}) = \sum_{i=1}^{n} \rho(y_i - \vec{x}_i^T \vec{\beta}) = \sum_{i=1}^{n} \rho(r_i)$$

where ρ is a real-valued **loss function** (in the OLS case, this was simply the square function). r_i is our residual for observation i.
Taking the derivative

$$\begin{aligned} \frac{dS(\vec{\beta})}{d\vec{\beta}} &= \sum_{i=1}^{n} \rho'(y_i - \vec{x}_i^T \vec{\beta})(-1)\vec{x}_i^T \\ &= -\sum_{i=1}^{n} \rho'(r_i)\vec{x}_i^T \end{aligned}$$

Solving for the extremum we have

$$\sum_{i=1}^{n} \phi(r_i)\vec{x}_i^T = \vec{0}^T$$

where $\phi(r) = \rho'(r)$ (derivative with respect to $\vec{\beta}$).

Remark 5.1 (LSE)**.** If $\rho(r) = r^2$ we get LSE, that is ($\phi(r) = 2r$)

$$\begin{aligned} \vec{0} &= \sum_{i=1}^{n} 2r\vec{x}_i \\ &= 2\sum_{i=1}^{n} (\vec{x}_i y_i - \vec{x}_i^T \vec{x}_i \vec{\beta}) \\ &= 2(X^T Y - X^T X\vec{\beta}) \end{aligned}$$

which exactly solves to our LSE closed form solution.

5.2 Discrepancy function and log-likelihood

Let us compare our discrepancy function with the log-likelihood for linear models:

$$\begin{aligned} l(\vec{\beta}) &= \sum_{i=1}^{n} l_i(\vec{\beta}) \\ &= \sum_{i=1}^{n} l(r_i) \end{aligned}$$

where $l(r_i) = \frac{-r_i^2}{2\sigma^2}$, a function only of r_i.
The second equality follows from the following remark:

Remark 5.2. Note $l_i(\vec{\beta})$ is the ith observation's contribution to $l(\vec{\beta})$ i.e.

$$l_i(\vec{\beta}) = \log f(y_i \mid \vec{x}_i^T\vec{\beta}, \sigma^2)$$

For a linear model we have

$$f(y_i \mid \vec{x}_i^T\vec{\beta}, \sigma^2) \sim N(\vec{x}_i^T\vec{\beta}, \sigma^2)$$

so $l_i(\vec{\beta}) = -\frac{r_i^2}{2\sigma^2} + C$ where $C = -\frac{1}{2}\log(2\pi) - \log\sigma$ a constant.
We let $l(r_i) = -\frac{r_i^2}{2\sigma^2}$. Since the constant does not change with respect to β we can omit it from our objective function.

From above we observe that minimizing the discrepancy function is the same as maximizing the log likelihood where $\rho(r) = -l(r)$ in the discrepancy function.

Definition 5.1 (M-estimator)**.** We call the estimator $\vec{\beta}$ that minimizes $\sum_{i=1}^{n}\rho(r_i)$ the **M-estimator** or the **maximum-likelihood type estimator**.

5.3 Iteratively re-weighted least squares (IRLS)

Note that the solution turns out to be a *WLS estimator*:

$$\begin{aligned} \vec{0} &= \sum_{i=1}^{n} \phi(r_i)\vec{x}_i \\ &= \sum_{i=1}^{n} \frac{\phi(r_i)}{r_i} r_i\vec{x}_i \\ &= \sum_{i=1}^{n} w(r_i)(y_i - \vec{x}_i^T\vec{\beta})\vec{x}_i \\ &= \sum_{i=1}^{n} w_i(y_i - \vec{x}_i^T\vec{\beta})\vec{x}_i \end{aligned}$$

where we let $w_i = w(r_i) = \frac{\phi(r_i)}{r_i}$. If we solve this we see that the solution is WLS where

$$\hat{\vec{\beta}} = (X^TWX)^{-1}X^TWY$$

with $W = \text{diag}(w_1, \ldots, w_n)$.

However, the weights of this WLS depend on the residuals which in turn depends on $\vec{\beta}$. If we are given an initial estimate of $\vec{\beta}^{(0)}$, we could *iteratively update residuals* and $\vec{\beta}$ to converge to a solution. We proceed as follows:

Initialization Initialization: set $j = 0$

Step 1 Compute residuals

$$\hat{r_i}^{(j)} = y_i - \vec{x}_i^T \hat{\vec{\beta}}^{(j)} \qquad i = 1, \ldots, n$$

Step 2 Update weights

$$w_i^{(j)} = \frac{\phi(\hat{r}_i^{(j)})}{\hat{r}_i^{(j)}}$$

and let $W^{(j)} = \text{diag}(w_1^{(j)}, \ldots, w_n^{(j)})$.

Step 3 WLS to estimate next set of $\hat{\vec{\beta}}^{(j+1)}$

$$\hat{\vec{\beta}}^{(j+1)} = (X^T W^{(j)} X)^{-1} X^T W^{(j)} Y$$

Step 4 Set $j = j + 1$ and return to Step 1 if convergence criterion is not met.

We can this procedure **iteratively re-weighted least squares (IRLS)**.
The convergence criterion is typically

$$\|\hat{\vec{\beta}}^{(j+1)} - \hat{\vec{\beta}}^{(j)}\| \leq \epsilon$$

with the L2/Euclidean norm and for some small positive constant ϵ.

5.4 Why IRLS?

Question 5.1. Why do we need to use iteratively re-weighted least squares?
In ordinary least squares with Gaussian response and loss function r_i^2, there is no reason to use IRLS since OLS and IRLS are equivalent (the loss function r_i^2 simplifies IRLS to OLS).
However in **generalized linear models (GLMs)** (STAT 431/831) we may have a different type of response (e.g. Bernoulli 0/1 or categorical) and thus we may define our loss function $\rho(r_i)$ differently.
We may also want to modify our $\rho(r_i)$ to de-emphasize huge outliers (see next section).

5.5 Robust regression

Robust regression tries to de-emphasize the influence of large outliers.

Question 5.2. What loss function ρ (and ϕ) should we use?
In ordinary least squares (OLS) we can use

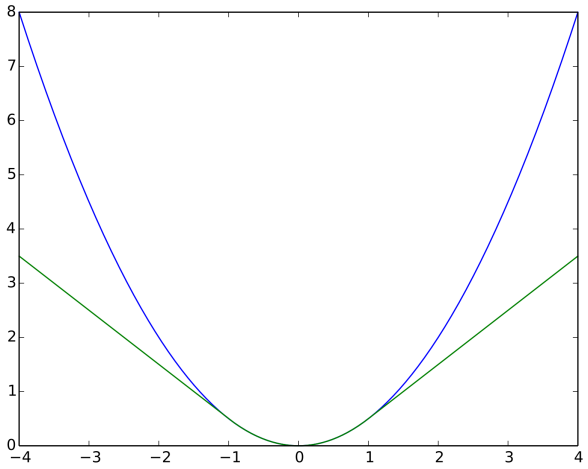
$$\rho(r) = \frac{1}{2} r^2$$
$$\phi(r) = r$$
$$w(r) = \frac{\phi(r)}{r} = 1$$

so we essentially have $W = I_{n \times n}$ which devolves into OLS as expected.

Remark 5.3. The residual function for OLS is unbounded and so extreme outliers with large residuals have significantly more influence.
Huber (1964) proposed a modified loss function (**Huber loss**) which de-emphasizes outliers:

$$\rho(r) = \begin{cases} \frac{1}{2}r^2 & \text{if } |r| \leq c \\ c(|r| - \frac{1}{2}c) & \text{if } |c| > c \end{cases}$$

The modified loss function essentially makes the loss function linear after a certain threshold c:



We also let

$$\phi(r) = \begin{cases} r & \text{if } |r| \leq c \\ c\text{sign}(r) & \text{if } |c| > c \end{cases}$$

and thus

$$w(r) = \begin{cases} 1 & \text{if } |r| \leq c \\ \frac{c}{|r|} & \text{if } |c| > c \end{cases}$$

The ϕ and weight w functions look like

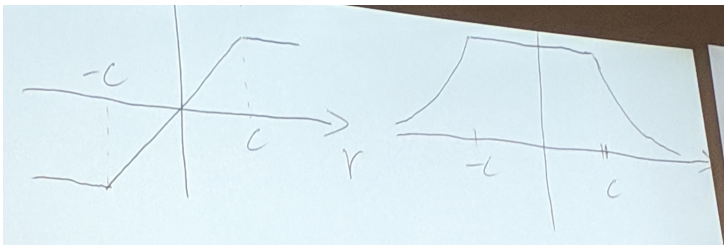


Figure 5.1: Left: $\phi(r)$. Right: $w(r)$ for Huber's loss function.

How do we decide c? Huber suggested $c = 1.345$ and showed it achieved 95% of LSE asymptotically when the true distribution is normal (95% efficiency essentially means the the variance of the betas from OLS is 95% that of the variance of the betas using Huber's loss).

Question 5.3. Since c is fixed, what if our residuals are scaled to very large or small values (e.g. $O(1e5)$ or $O(1e-4)$)? We would have to scale our data beforehand to make it within a sensible range so that $c = 1.345$ makes sense.

Sometimes we prefer the ϕ function to "redescend" i.e. $\phi(r) \to 0$ when $|r|$ is large (that is: we fully de-emphasize outliers). Other ϕ functions include

Redescending M-estimator (Hampel)

$$\phi(r) = \begin{cases} r & \text{if } 0 \le |r| \le a \\ a\text{sign}(r) & \text{if } a \le |r| \le b \\ a\frac{c-|r|}{c-b}\text{sign}(r) & \text{if } b \le |r| \le c \\ 0 & \text{if } |r| > c \end{cases}$$

The recommended settings are $a = 2, b = 4, c = 8$ (with appropriately scaled data and residuals).

Tukey's biweight

$$\phi(r) = \begin{cases} r\left(1 - \left(\frac{r}{c}\right)^2\right)^2 & \text{if } |r| \le c \\ 0 & \text{if } |r| > c \end{cases}$$

where $c = 4.685$ is typically used. This is designed to have 95% efficiency as well for a true normal distribution.

6 January 29, 2019

6.1 Remark on robust regression and constants

Remark 6.1. All recommended constants in the various robust regression methods (Huber, Hampel, Tukey) are based on the assumption that $Var(r) = 1$. Therefore in practice we typically need to scale the residuals i.e. $r_i' = \frac{r_i}{s}$ where s is a scale parameter.
One simple solution is to estimate the **median absolute deviation (MAD)**:

$$\text{MAD} = \text{median}(|r_i|)$$

and let $\hat{s} = \frac{\text{MAD}}{0.6745}$. For the standard normal distribution we note that MAD $= 0.6745$.

6.2 Sensitivity curve and breakdown point

Let $T_n(y_1, \ldots, y_n)$ be a population attribute (that is a function of the same points). To see how **sensitive** T_n is to an individual data point, define

$$SC(y) = \frac{T_n(y_1, \ldots, y_{n-1}, y) - T_{n-1}(y_1, \ldots, y_{n-1})}{\frac{1}{n}}$$

which is the difference between $T_n(\cdot)$ (with all n points) and $T_{n-1}(\cdot)$ (with one point y omitted) compare to the contamination size $\frac{1}{n}$.

Example 6.1. Let $T_n(y_1, \ldots, y_n) = \frac{1}{n}\sum_{i=1}^n y_i = \bar{y}_n$ (sample mean).
Note that

$$T_n = \sum_{i=1}^{n-1} y_i + y = \frac{n-1}{n}\bar{y}_{n-1} + y$$

Note that $SC(y)$ is simply

$$\begin{aligned} SC(y) = n(T_n - T_{n-1}) &= (n-1)\bar{y}_{n-1} + y - n\bar{y}_{n-1} \\ &= y - \bar{y}_{n-1} \end{aligned}$$

Definition 6.1 (Breakdown point)**.** *Informally*, the **breakdown point** of a statistic is the largest proportion of contamination before the statistic breaks down.
Formally, let $\vec{z}_i = (x_{i1}, x_{i2}, \ldots, x_{ip}, y_i)^T$ for $i = 1, \ldots, n$ be the ith data vector.
Let $Z = (\vec{z}_1, \ldots, \vec{z}_n)$ be the whole set. Let T be the statistic of intrest. The *worst error* for swapping m z_i's is

$$e(m; T, Z) = \sup_{Z_m^*} \|T(Z_m^*) - T(Z)\|$$

where Z_m^* is Z with any of its m data vectors replaced.
The **breakdown point** is then defined as

$$\min \left\{ \frac{m}{n} \mid e(m; T, Z) = \infty \right\}$$

Remark 6.2. That is: the breakdown point measures the minimum **proportion** of points required to influence the statistic *significantly*.

Some breakdown point examples:

Sample mean Note we can simply swap out $m = 1$ point arbitrarily such that $e(1; T, Z) \to \infty$ thus the breakdown point is $\frac{1}{n} \to 0$ as $n \to \infty$.

Median The breakdown point is $\frac{1}{2}$ as $n \to \infty$: we need to change at least half of them to aribitrarily influence the median e.g. make it go to infinity.

$k\%$ **trimmed mean** The $k\%$ trimmed mean is defined as the mean after discarding the lowest $k\%$ and highest $k\%$ of y_i's.

Breakdown point is $k\%$ (we swap out the top $k\% + 1$ points).

6.3 Least median squares (LMS)

Recall for regression, the LSE of $\vec{\beta}$ is

$$\text{argmin}_{\vec{\beta}} \sum_{i=1}^{n} (y_i \vec{x}_i^T \vec{\beta})^2$$

or equivalently

$$\text{argmin}_{\vec{\beta}} \text{average}(y_i \vec{x}_i^T \vec{\beta})^2$$

To make it robust for "outliers" or contaminations i.e. to ensure we have a *high breakdown point* we could consider the **least median squares (LMS) estimator**:

$$\vec{\beta}_{LMS} = \text{argmin}_{\vec{\beta}} \text{median}(y_i \vec{x}_i^T \vec{\beta})^2$$

which has a breakdown point of $\frac{1}{2}$ (compared to a breakdown point of $\frac{1}{n}$ for OLS).

6.4 Least trimmed average sum of squares (LTS)

Similar to how we made our objective function for OLS more robust by considering the median in LMS, we can also consider the **(least) trimmed average sum of squares (LTS) estimator**:

$$\vec{\beta}_{LTS} = \text{argmin}_{\vec{\beta}} \sum_{i=1}^{k} r^2_{(i)}$$

where $r^2_{(i)}$ is the ith smallest squared residual.
Note the breakdown point for LTS is $\frac{n-k+1}{n}$ (compared to a breakdown point of $\frac{1}{n}$ for OLS).

7 January 31, 2019

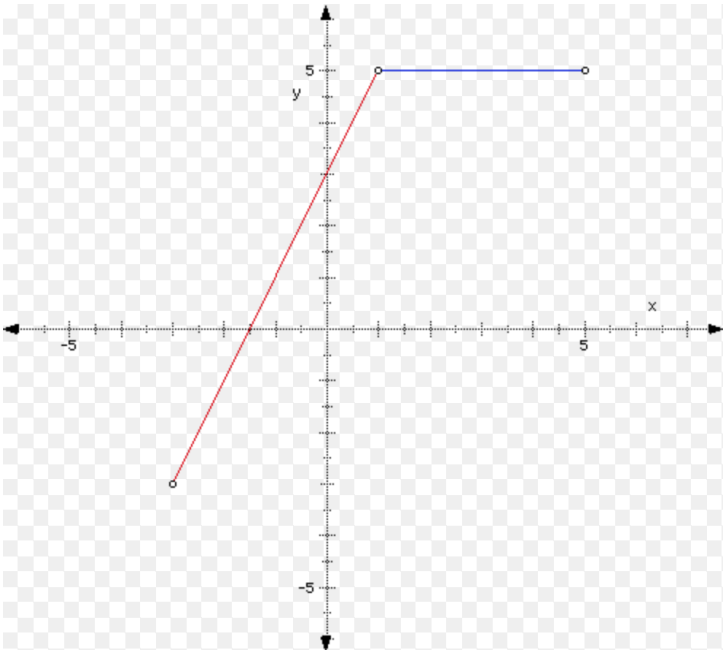
8 Local linear regression with k-nearest neighbours

Instead of fitting one linear regression model with all points, we can instead fit local linear regression models for neighbourhoods of points. In essence we are fitting piecewise linear functions.
We first look at **piecewise polynomials** and **splines**.

8.1 Piecewise polynomials (splines)

Definition 8.1 (Spline)**.** We collectively call functions that aim to interpolate and smooth over some distribution **splines**. Piecewise polynomials are a common choice for splines.

For continuous piecewise polynomial functions, the simplest form is **piecewise linear** (as seen before):



which can be specified as a single linear model

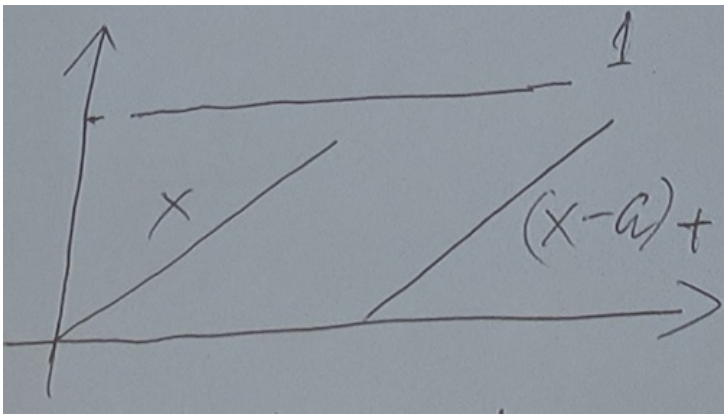
$$f(x) = \beta_0 + \beta_1 x + \beta_2 (x - a) I(x \geq a)$$

Remark 8.1. Piecewise linear is also called the **broken stick** method.

For notation simplicity let us define $(x)_+ = \max(x, 0)$ such that we have

$$f(x) = \beta_0 + \beta_1 x + \beta_2 (x - a)_+$$

Thus our basis functions are $1, x, (x-a)_+$. Here is plot of the basis:



This is an example of the **truncated power series**. We can easily generalize this model to accomodate many break points or knots.
However, picewise linear functions are *not differentiable* at their break points since $f'(x)$ is not continuous.
Recall that for a **piecewise quadratic function** we have

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 (x - a)_+^2$$

where our basis functions are $1, x, x^2, (x-a)_+^2$. Note that a piecewise quadratic model $f(x)$ is indeed differentiable at the break points.

8.2 Cubic splines

Remark 8.2. The most commmonly used spline is the **cubic spline**, which is piecewise cubic where $f(x), f'(x), f''(x)$ are all continuous.

Let $t_1 < t_2 < \ldots, t_k$ be fixed and known knots, where t_1 and t_k are boundary knots and $t_2, \ldots, t_{k-1}$ are interior knots.
Then the basis consists of the functions $1, x, x^2, x^3, (x-t_1)_+^3, \ldots, (x-t_k)_+^3$. That is any **cubic spline** with the above k knots can be expressed as

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{j=1}^{k} \beta_{j+3} (x - t_j)_+^3$$

Remark 8.3.

1. There are $k + 4$ parameters.
2. $f(x)$ is continuous up to the 2nd derivative.

Proof. This is obviously true between knots. We verify at $x = t_i$:

$$f(t_i) = \beta_0 + \beta_1 t_i + \beta_2 t_i^2 + \beta_3 t_i^3 + \sum_{j=1}^{i-1} \beta_{j+3}(t_i - t_j)_+^3$$

note that $(x - t_j)_+^3 = 0$ for $x < t_{i+1}$ and $j = i + 1, \ldots, k$.

Note that $\lim_{x \to t_i^-} f(x) = f(t_i)$ since $(x - t_i)_+ = 0$ if $x < t_i$ so $\lim_{x \to t_i^-}(x - t_i)_+^3 = 0$.

Also $\lim_{x \to t_i^+} f(x) = f(t_i)$ since $\lim_{x \to t_i^+}(x - t_i)_+^3 = 0$.

Therefore $\lim_{x \to t_i^-} f(x) = \lim_{x \to t_i^+} f(x) = f(t_i)$ so f is continuous at t_i for all $i = 1, \ldots, k$.

Similarly we can show this for $f'(x)$ and $f''(x)$. □

9 February 5, 2019

9.1 Natural cubic splines (NCS)

A cubic spline is called a **natural cubic spline** with knots $\{t_1, \ldots, t_k\}$ if $f(x)$ is linear when $x \notin [t_1, t_k]$, that is

$$f(x) = \begin{cases} t_0(x) = a_0 + b_0 x & \text{if } x < t_1 \\ t_k(x) = a_k + b_k x & \text{if } x > t_k \end{cases}$$

Question 9.1. How many free parameters are there in the natural cubic spline?

Answer. Note that in general cubic splines, we have $k + 4$ parameters. If we constrain our spline to be linear at both ends ($x < t_1$ and $x > t_k$) then we essentially remove the quadratic and cubic terms and thus parameters at each end. So we remove 4 parameters and thus we have k free parameters.

To express an NCS, note that for a regular cubic spline we have

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \sum_{j=1}^{k} \beta_{j+3}(x - t_j)_+^3$$

Secondly our constraints are:

$f(x)$ **is linear when** $x < t_1$ We know that $\beta_4, \ldots, \beta_k + 3$ are already 0 when $x < t_1$.

Thus we need only specify that $\beta_2 = \beta_3 = 0$.

$f(x)$ **is linear when** $x > t_k$ We require that

$$\sum_{j=1}^{k} \beta_{j+3} = 0$$
$$\sum_{j=1}^{k} \beta_{j+3} t_j = 0$$

The conditions are necessary (proof left as assignment question).

Note that we have 4 separate (linearly independent) constraints on the parameters hence why we lose 4 degrees of freedom.
Let $d_j(x) = \frac{(x-t_j)_+^3 - (x-t_k)_+^3}{t_k - t_j}$, then NCS can be expressed as linear combination of the basis functions

$$\begin{aligned} N_0(x) &= 1 \\ N_1(x) &= x \\ N_i(x) &= (t_k - t_j)\big[d_i(x) - d_1(x)\big] \qquad i = 2, \ldots, k-1 \end{aligned}$$

More conveniently we can exxpress the NCS as

$$f(x) = \sum_{j=1}^{k} \beta_j N_j(x)$$

where $N_1(x) = 1, N_2(x) = x$ and $N_j(x) = d_{j-1}(x) - d_1(x)$ for $j = 3, \ldots, k$.

Remark 9.1.

1. If $x < t_1$, then $d_j(x) = 0 \Rightarrow N_j(x) = 0$ for $j = 3, \ldots, k$.
2. If $x > t_k$, then $d_j(x) = \frac{(x-t_j)^3 - (x-t_k)^3}{t_k - t_j}$ reduces to a quadratic function of x where the coefficient of x^2 term is 3.

   Since $N_j(x) = d_{j-1}(x) - d_1(x)$ then it is a linear function of x if $x > t_k$ for $j = 3, \ldots, k$.

Definition 9.1 (Regression splines)**.** The fixed-knot splines, such as cubic splines and NCS, are called **regression splines**.

9.2 Fitting NCS

Let $y_i = f(x_i) + \epsilon_i$ for some response y_i and explanatory variates x_i and some arbitrary continuous function $f(\cdot)$. We can approximate/regress $f(x)$ by $\sum_{j=1}^{k} \beta_j N_j(x)$ (NCS) i.e.

$$y_i \approx \sum_{j=1}^{k} \beta_j N_j(x_i) + \epsilon_i$$

Now we simply fit the following linear model with design matrix

$$X = \begin{bmatrix} N_1(x_1) & \ldots & N_k(x_1) \\ \vdots & \ddots & \vdots \\ N_1(x_n) & \ldots & N_k(x_n) \end{bmatrix}$$

where

$$\beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

Remark 9.2. The problem becomes a regular regression problem with design matrix generated from the basis functions N_j's.

9.3 General function fitting with basis funcitons

We extend our method for fitting NCS: more generally for a p-dimensional input vector $\vec{x}$, we can consider the following appproximation to $f(\vec{x})$

$$f(\vec{x}) = \sum_{j=1}^{k} \beta_j h_j(\vec{x})$$

where $\{h_j\}$ are a series of basis functions.

That is: we approximate $f(\vec{x})$ as a linear basis expansion. Then we form the design matrix $X = \left[h_j(\vec{x}_i)\right]$ where i indexes the row (ith sample) and j indexes the column (jth basis function).
Some examples:

1. $h_j(\vec{x}) = x_j$ for $j = 1, \ldots, p$ is the original linear model where basis functions are the jth component
2. $h_j(\vec{x}) = \log(x_j)$ are arbitrary transformations
3. $h_j(\vec{x}) = x_j^k$ for $k \in \mathbb{N}$ is polynomial regression
4. $h_j(\vec{x}) = N_j(\vec{x})$ is NCS

10 February 7, 2019

10.1 Choosing k for NCS

Recall that the basis functions for NCS are

$$\begin{aligned} N_0(x) &= 1 \\ N_1(x) &= x \\ N_i(x) &= d_{j-1}(x) - d_1(x) \qquad j = 3, \ldots, k \end{aligned}$$

We still need to choose a k and our knots $t_1, \ldots, t_k$.
Some examples of how to choose k and knots:

Equal-distance knots We choose k first arbitrarily e.g. $k = 5$, then we use an equal-distance grid between the min and max of x_i's.

Quantiles **Quantiles** are also a popular choice e.g. $\frac{i}{k-1}$ quantiles for each x_i, $i = 0, \ldots, k-1$.

Degrees of freedom Alternatively we can instead specify the degrees of freedom for an NCS i.e. the number of free parameters i.e. the number of knots. Usually knots are placed at equal distance quantiles.

10.2 Smoothing splines

Consider the following **penalized** regression problem

$$\hat{f}_\lambda(x) = \text{argmin}_f \sum_{i=1}^{n} [y_i - f(x_i)]^2 + \lambda \int_{-\infty}^{\infty} [f''(x)]^2 \, \mathrm{d}x$$

Remark 10.1.

1. $\sum_{i=1}^{n}[y_i - f(x_i)]^2$ is the sum of squared residuals which measures the goodness of fit.
2. $\int_{-\infty}^{\infty}[f''(x)]^2\,\mathrm{d}x$ measures the "roughness" of $f(x)$.

   Remark 10.2. Note that we try to minimize the integral over the $f''(x)$ (squared), which is essentially minimizing $f''(x)$ so that it is close to 0.

   For example, if $f(x) = \beta_0 + \beta_1 x$ (OLS) then $f''(x) = 0$ thus $\int_{-\infty}^{\infty}[f''(x)]^2 = 0$ i.e. no penalty for OLS.
3. The role of λ: if $\lambda = 0$ then we have no roughness penalty and we will minimize the SSR over all functions and $\hat{f}_\lambda(x)$ is the interpolating line.

   If $\lambda = \infty$ then we will force $\int_{-\infty}^{\infty}[f''(x)]^2\,\mathrm{d}x = 0$ thus $\hat{f}_\lambda(x)$ is the ordinary least square fit.
4. Remarkably we can show that $\hat{f}_\lambda(x)$ is just the natural cubic spline with knots at distinct values of $\{x_i\}_{i=1}^n$.
5. NCS is the "smoothest" interpolator.

   For any complex function $f(x)$ if we only know the value of k points $\{f(t_i)\}_{i=1}^k$ then we can use $\{t_i, f(t_i)\}_{i=1}^k$ to determine an NCS $s(x)$ such that $s(t_i) = f(t_i)$ for $i = 1, \ldots, k$.

   Claim.
   $$\int_{-\infty}^{\infty}[s''(x)]^2\,\mathrm{d}x \leq \int_{-\infty}^{\infty}[f''(x)]^2\,\mathrm{d}x$$

Definition 10.1 (Smoothing spline)**.** We call the function fitted by the penalized regression a **smoothing spline**.

We determine the β for the NCS smoothing spline. Note that

$$\hat{f}_\lambda(x) = \sum_{j=1}^{k}\beta_j N_j(x)$$

that is

$$\hat{\beta}_\lambda = \mathrm{argmin}_f \sum_{i=1}^{n}[y_i - \sum_{j=1}^{k}\beta_j N_j(x)]^2 + \lambda\int_{-\infty}^{\infty}[\sum_{j=1}^{k}\beta_j N_j''(x)]^2\,\mathrm{d}x$$

Note that we can re-express this in matrix notation where

$$\sum_{i=1}^{n}[y_i - \sum_{j=1}^{k}\beta_j N_j(x)]^2 = (Y - X\vec{\beta})^T(Y - X\vec{\beta})$$

where

$$X = \begin{bmatrix} N_1(x_1) & \ldots & N_k(x_1) \\ \vdots & \ddots & \vdots \\ N_1(x_n) & \ldots & N_k(x_n) \end{bmatrix}$$

Also

$$\begin{aligned}
\int_{-\infty}^{\infty}[\sum_{j=1}^{k}\beta_j N_j''(x)]^2\,\mathrm{d}x &= \int_{-\infty}^{\infty}[\sum_{j=1}^{k}\beta_j N_j''(x)][\sum_{l=1}^{k}\beta_l N_l''(x)]\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}[\sum_{j=1}^{k}\sum_{l=1}^{k}\beta_j\beta_l N_j''(x)N_l''(x)]\,\mathrm{d}x \\
&= \sum_{j=1}^{k}\sum_{l=1}^{k}\beta_j\beta_l\frac{\int_{-\infty}^{\infty}N_j''(x)N_l''(x)\,\mathrm{d}x}{N_{jl}} \qquad N_{jl} \text{ some constant} \\
&= \vec{\beta}^T N\vec{\beta}
\end{aligned}$$

where $N = (N_{jl})$ (i,j-th entry is N_{jl}).
Therefore we can let

$$\begin{aligned}
S(\vec{\beta}) &= (Y - X\vec{\beta})^T(Y - X\vec{\beta}) + \lambda\vec{\beta}^T N\vec{\beta} \\
&= Y^TY - \vec{\beta}^TX^TY - Y^TX\vec{\beta} + \vec{\beta}^TX^TX\vec{\beta} + \lambda\vec{\beta}^TN\vec{\beta} \\
&= Y^TY - 2Y^TX\vec{\beta} + \vec{\beta}^T(X^TX + \lambda N)\vec{\beta}
\end{aligned}$$

and $\hat{\vec{\beta}}_\lambda = \text{argmin}S(\vec{\beta})$.
Recall that for matrix Y, A and vector $\vec{c}$

$$\begin{aligned}
\frac{\partial\vec{c}^TY}{\partial Y} &= \vec{c}^T \\
\frac{\partial Y^TAY}{\partial Y} &= 2Y^TA^T
\end{aligned}$$

thus we have

$$\begin{aligned}
&\frac{\partial S(\vec{\beta})}{\partial\vec{\beta}} = 0 = -2Y^TX + 2\vec{\beta}^T(X^TX + \lambda N)^T \\
\Rightarrow&(X^TX + \lambda N)\hat{\vec{\beta}}_\lambda = X^TY \\
\Rightarrow&\hat{\vec{\beta}}_\lambda = (X^TX + \lambda N)^{-1}X^TY
\end{aligned}$$

To calculate the *effective number of parameters* or effective df (edf): recall for NCS we have k knots and in OLS with $X_{n\times p}$

$$\hat{Y} = HY = X^T(X^TX)^{-1}X^TY$$

where the number of parameters is $df = tr(H)$.
Now in the smoothing spline, we have

$$\hat{Y}_\lambda = X^T(X^TX + \lambda N)^{-1}X^TY = A_\lambda Y$$

where the effective number of parameters is $df_\lambda = tr(A_\lambda)$.

Remark 10.3. When $\lambda\to\infty$, $df_\lambda \to 2$.