Lecture 3:

Maximum Likelihood Estimation (MLE), Linear Regression, Linear Models

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Bayesian Data Analysis and Machine Learning for Physical Sciences

Course Map

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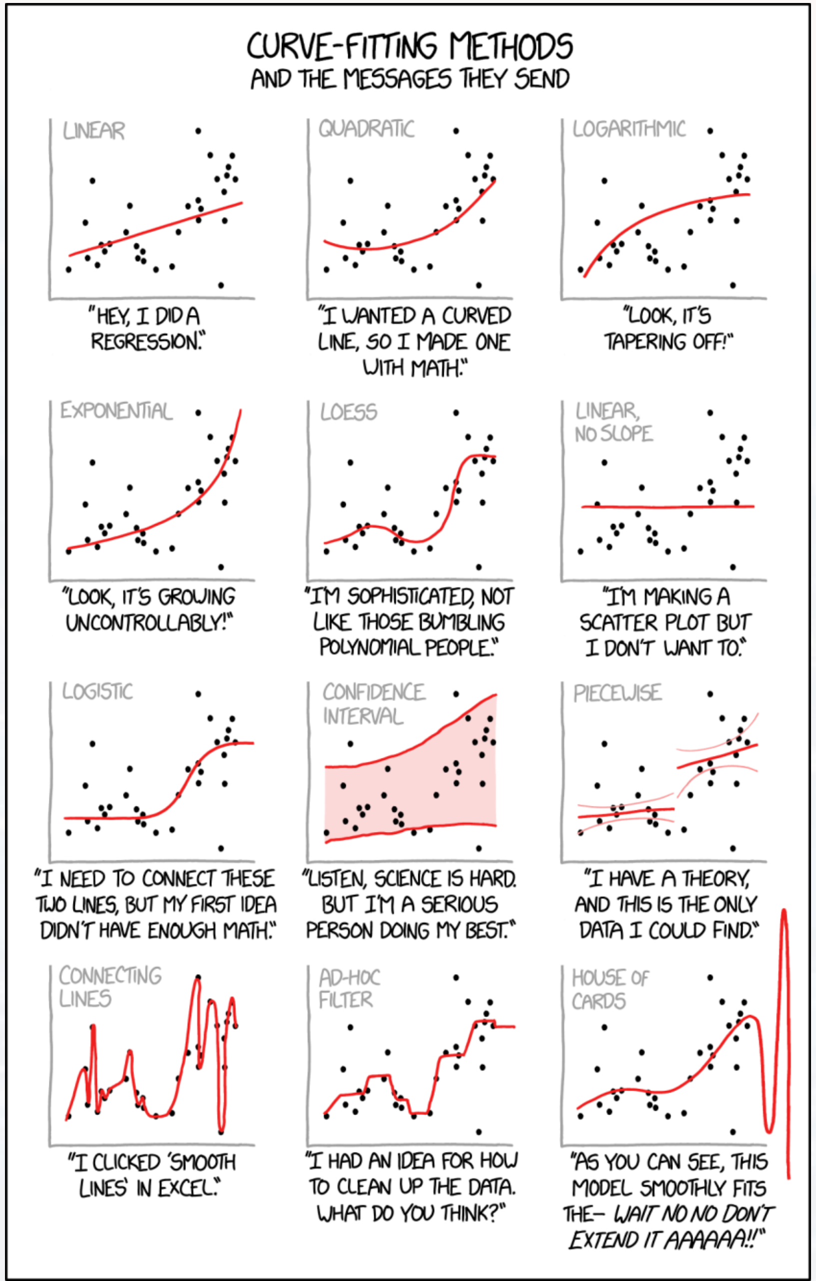
Maximum Likelihood Estimation, Linear Regression



<u>Outline</u>

Maximum Likelihood Estimation (MLE)

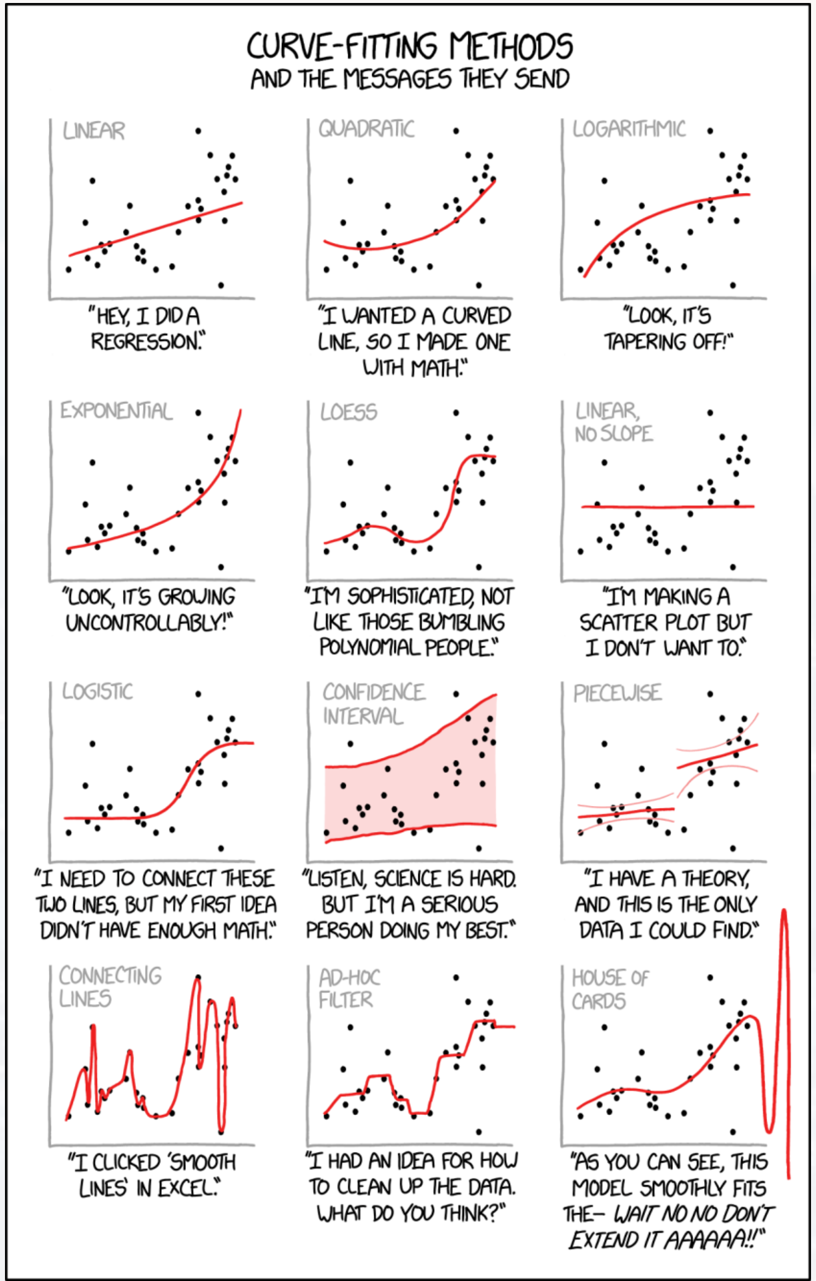
- idea
- examples

Linear Models

- classical model
- regularization
- extensions

Regression

Maximum Likelihood Estimation, Linear Regression



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Maximum Likelihood Estimation, Linear Regression:

Bayesian:

$$P(\theta|D) = \frac{\overbrace{\boxed{P(D|\theta)}}^{\text{likelihood function}}\overbrace{\boxed{P(\theta)}}^{\text{prior}}}{\underbrace{\boxed{P(D)}}_{\text{evidence (const wrt q)}}}$$

$$\int P(\theta|D)\ d\theta = 1$$

parameter θ

"Classical" approach: **M**aximum **L**ikelihood **E**stimation

$x = \{x_1, x_2, \dots x_i, \dots, x_N\}$ data set of N independent observations

$\theta = \{\theta_1, \theta_2, \dots \theta_i, \dots, \theta_M\}$ set of parameters θ

$\theta = q$ (binomial)
$\theta = \{\mu, \sigma^2\}$ (normal dist)

$f_i(\theta, x_i)$ distribution f_i from which x_i has been drawn

Maximum Likelihood Estimation, Linear Regression:

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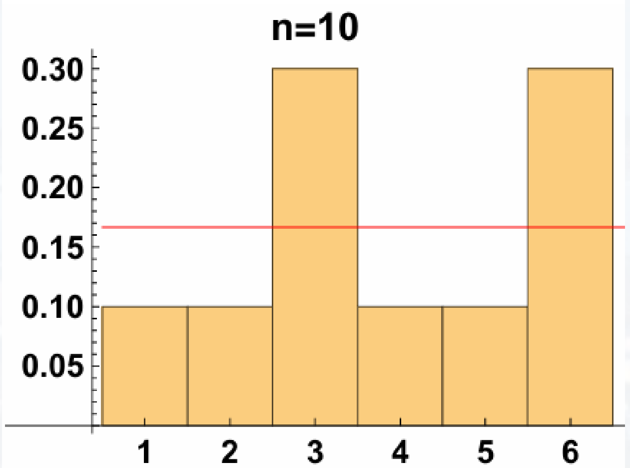
$f_i(\theta, x_i)$ distribution f_i from which x_i has been drawn

$L(\theta, x) = \prod_{i=1}^{N} f_i(\theta, x_i)$ joint density

goal: finding those $\hat{\theta}$ that maximize $L(\theta, x)$

$$\boxed{\hat{\theta} = \underset{\theta}{argmax}\{L(\theta, x)\}}$$

We aim to find the most likely one!



$\sigma = 2$, $\mu = 3.5$

$\sigma = 2$, $\mu = 5.0$

$\sigma = 1.5$, $\mu = 3.5$

$\sigma = 7.0$, $\mu = 1.0$

....and so on

Maximum Likelihood Estimation, Linear Regression:

<u>"Classical" approach:</u> **M**aximum **L**ikelihood **E**stimation

$$L(\theta, x) = \prod_{i=1}^{N} f_i(\theta, x_i)$$ joint density

goal: finding those $\hat{\theta}$ that maximize $L(\theta, x)$

$$\boxed{\hat{\theta} = \underset{\theta}{argmax}\{L(\theta, x)\}}$$

x: data set
θ: parameter
$f_i(\theta, x_i)$: density function

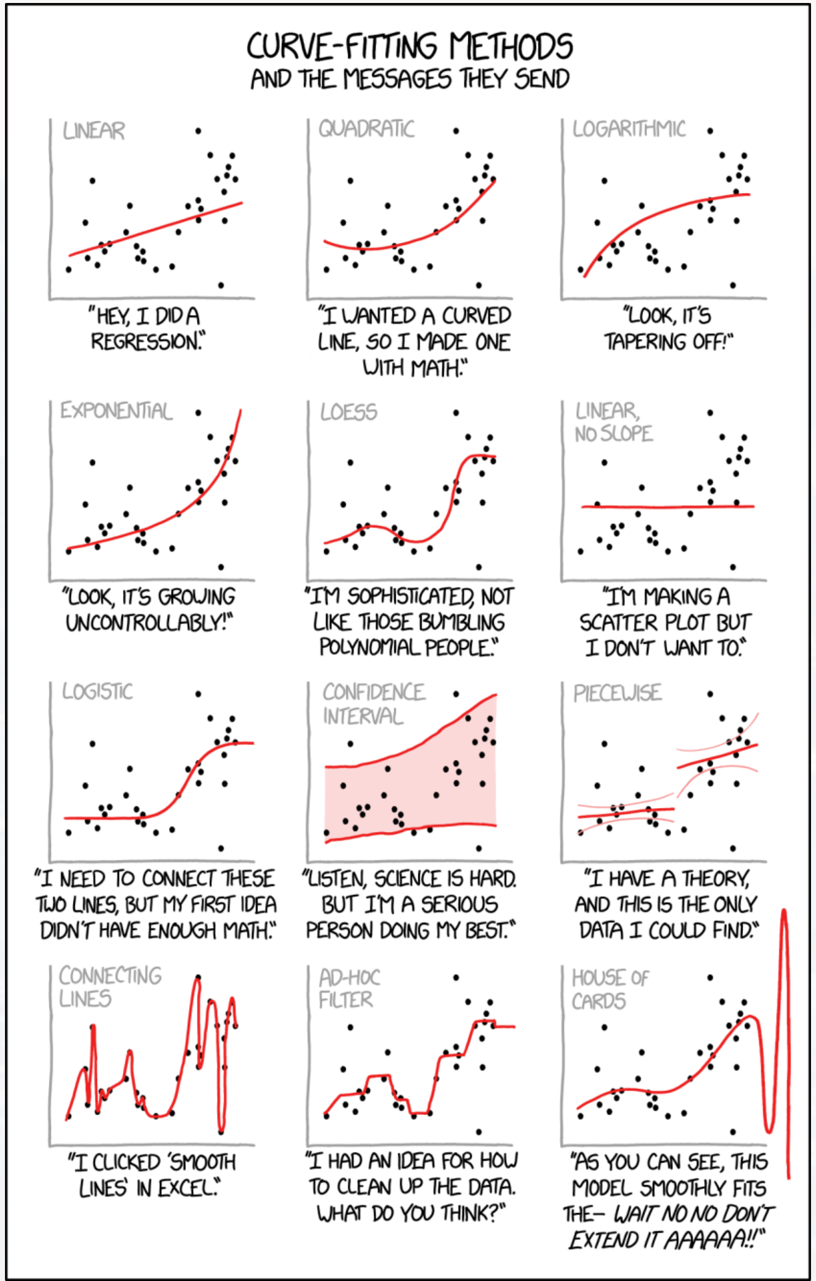
note:

- often we use $\mathrm{l}(\theta, x) = \ln[L(\theta, x)]$ for convenience
- we find $\hat{\theta}$ via $\frac{\partial L(\theta, x)}{\partial \theta_i} = 0$ for all θ_i
- equivalent to **MAP** assuming **an uniform prior**
- evaluate, if extreme is indeed a maximum:

  Hessian matrix $H = \left\{\frac{\partial^2\, \mathrm{l}(\theta, x)}{\partial \theta_i\, \partial \theta_j}\right\}$ has to be **locally** (around $\hat{\theta}$) **concave**

- we can add constrains using **Lagrangian Multipliers**

Maximum Likelihood Estimation, Linear Regression



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Maximum Likelihood Estimation, Linear Regression:

example I: binomial distribution

$x = \{HHTHTTT \ldots.\} \qquad \theta = q$

$f(q|x) = \binom{n}{k} \boxed{q^k(1-q)^{n-k}}$ equivalent to **MAP** assuming **an uniform prior** $\dfrac{P(D|\theta)P(\theta)}{P(D)}$

$$\frac{df}{dq} = \binom{n}{k} [kq^{k-1}(1-q)^{n-k} - q^k(n-k)(1-q)^{n-k-1}] = 0$$

ignoring $q = 1$ and $q = 0$: $\qquad k(1-q) = q(n-k) \qquad q_{best} = \dfrac{k}{n}$

$$\left.\begin{aligned} q_0 &= \frac{k}{n} \\ \sigma &= \sqrt{\frac{q_0(1-q_0)}{n}} \end{aligned}\right\} \quad q = \frac{k}{n} \pm \sqrt{\frac{q_0(1-q_0)}{n}}$$

last time:
Lagrange approximation from BPE

example II: normal distribution

$$x = \{x_1, x_2, \dots x_i, \dots, x_N\} \qquad \theta = \{\mu, \sigma^2\}$$

$$f_i(\theta, x_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{(x_i-\mu)^2}{\sigma^2}}$$

$$L(\theta, x) = \prod_{i=1}^{N} f_i(\theta, x_i) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i-\mu)^2}$$

$$l(\theta, x) = \ln[L(\theta, x)] = -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i - \mu)^2$$

$$\frac{\partial l(\theta,x)}{\partial \sigma} = -\frac{N}{\sigma} + \frac{1}{\sigma^3}\sum_{i=1}^{N}(x_i - \mu)^2 = 0$$

$$\boxed{\hat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}$$

example II: normal distribution

$$x = \{x_1, x_2, \ldots x_i, \ldots, x_N\} \qquad \theta = \{\mu, \sigma^2\}$$

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$$\frac{\partial l(\theta, x)}{\partial \mu} = \frac{1}{\sigma^2}\sum_{i=1}^{N}(x_i - \mu) = 0$$

$$\boxed{\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} x_i}$$

$$\boxed{\hat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}$$

Maximum Likelihood Estimation, Linear Regression:

example II: normal distribution

$$x = \{x_1, x_2, \dots x_i, \dots, x_N\} \qquad \theta = \{\mu, \sigma^2\}$$

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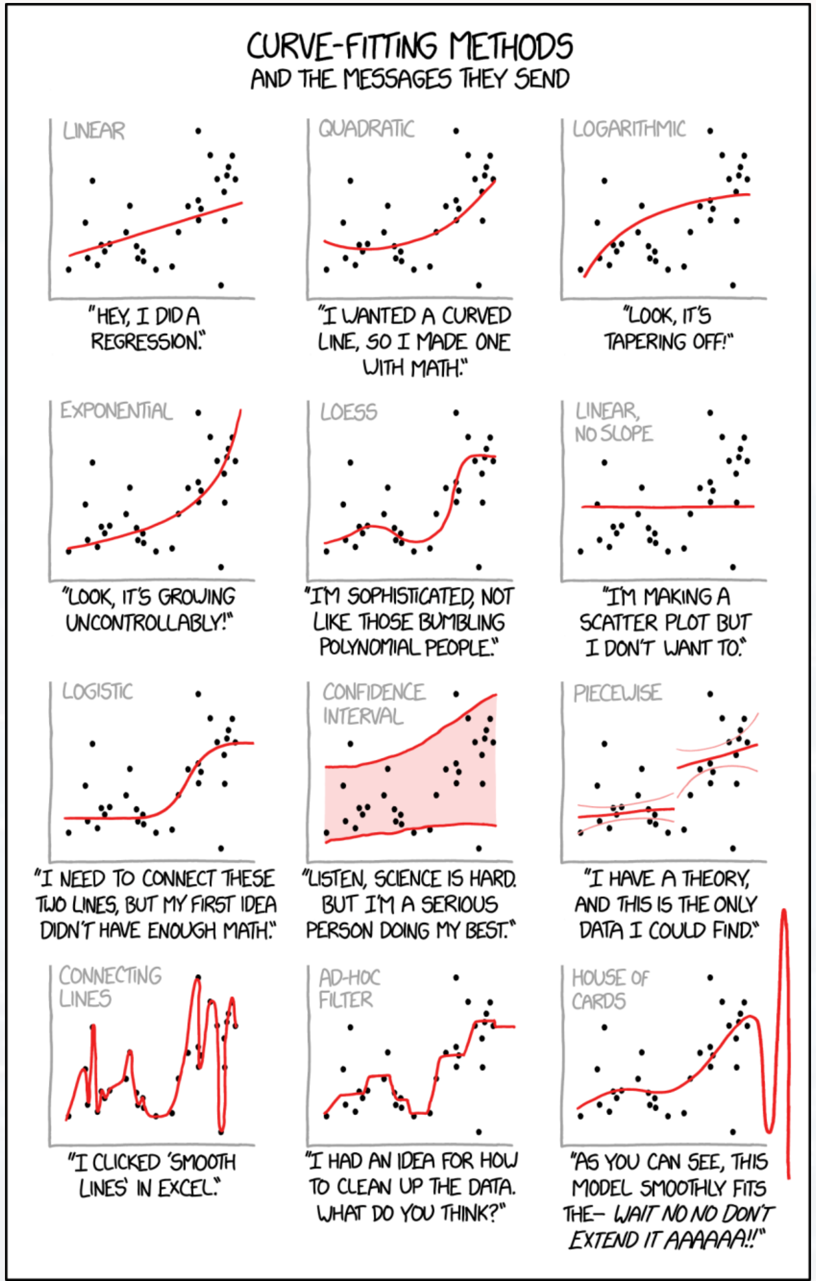
$$l(\theta, x) = \ln[L(\theta, x)] = -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(x_i - \mu)^2$$

$$\boxed{\hat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{\mu})^2}$$

$$\boxed{\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} x_i}$$

$$\hat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{\mu})^2 = \frac{1}{N}\sum_{i=1}^{N}\left(x_i - \frac{1}{N}\sum_{i=1}^{N} x_i\right)^2 = \frac{1}{N}\sum_{i=1}^{N} x_i{}^2 - \frac{1}{N^2}\sum_{i=1}^{N}\sum_{i=j}^{N} x_i\, x_j$$

Maximum Likelihood Estimation, Linear Regression



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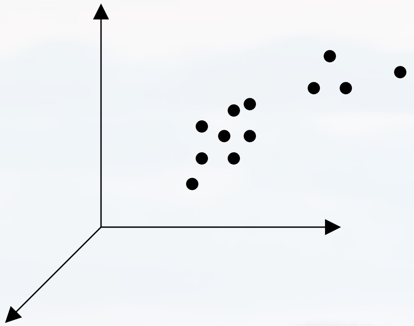
Maximum Likelihood Estimation, Linear Regression:

<u>idea:</u> data point y_k in N dimensional feature space



$y_k = f(x_1, \dots x_n, \dots x_N) + \epsilon_k$ for each data point k

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon_k$$

y:	**response**
x:	**regressors** (assumed to be independent)
β:	**factors** (how a regressor contributes to the response)
β_0:	**intercept**
ε:	**error** (stochasticity of the data, assumed to be normally dist.)

$$\underbrace{\begin{pmatrix} y_1 \\ \dots \\ y_k \\ \dots \\ \dots \\ y_K \end{pmatrix}}_{\text{Y}} = \underbrace{\begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1n} & \dots & x_{1N} \\ \dots & \dots & & & \dots & & \\ 1 & x_{k1} & & & x_{kn} & & \\ 1 & \dots & & & \dots & & \\ 1 & x_{K1} & x_{K2} & \dots & x_{Kn} & \dots & x_{KN} \end{pmatrix}}_{\text{X}} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_n \\ \dots \\ \beta_N \end{pmatrix}}_{\beta} + \underbrace{\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_k \\ \dots \\ \varepsilon_K \end{pmatrix}}_{\varepsilon}$$

$$\boxed{Y = X\beta + \varepsilon}$$

Maximum Likelihood Estimation, Linear Regression:

$$Y = X\beta + \varepsilon$$

***y*:**	**response**
***x*:**	**regressors** **(assumed to be independent)**
β:	**factors** **(how a regressor contributes to the response)**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error** **(stochasticity of the data, assumed to be normally dist.)**

classical model
regularizations
extensions

<u>fitting:</u> finding the best β in terms of minimizing the errors

$$(Y - X\beta)^T(Y - X\beta) = \sum_k {\varepsilon_k}^2$$

$$\frac{\partial}{\partial\beta}\sum_k {\varepsilon_k}^2 = 0$$

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

the model

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

X and *Y* are all observables

hat matrix $\mathrm{H} \coloneqq \boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T$

$H = H^T$ (symmetry)

$HH = H \rightarrow H^n = H$ (idempotency)

$$Y = X\beta + \varepsilon$$

y:	**response**
x:	**regressors (assumed to be independent)**
β:	**factors (how a regressor contributes to the response)**
β_0:	**intercept**
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evaluating the result:

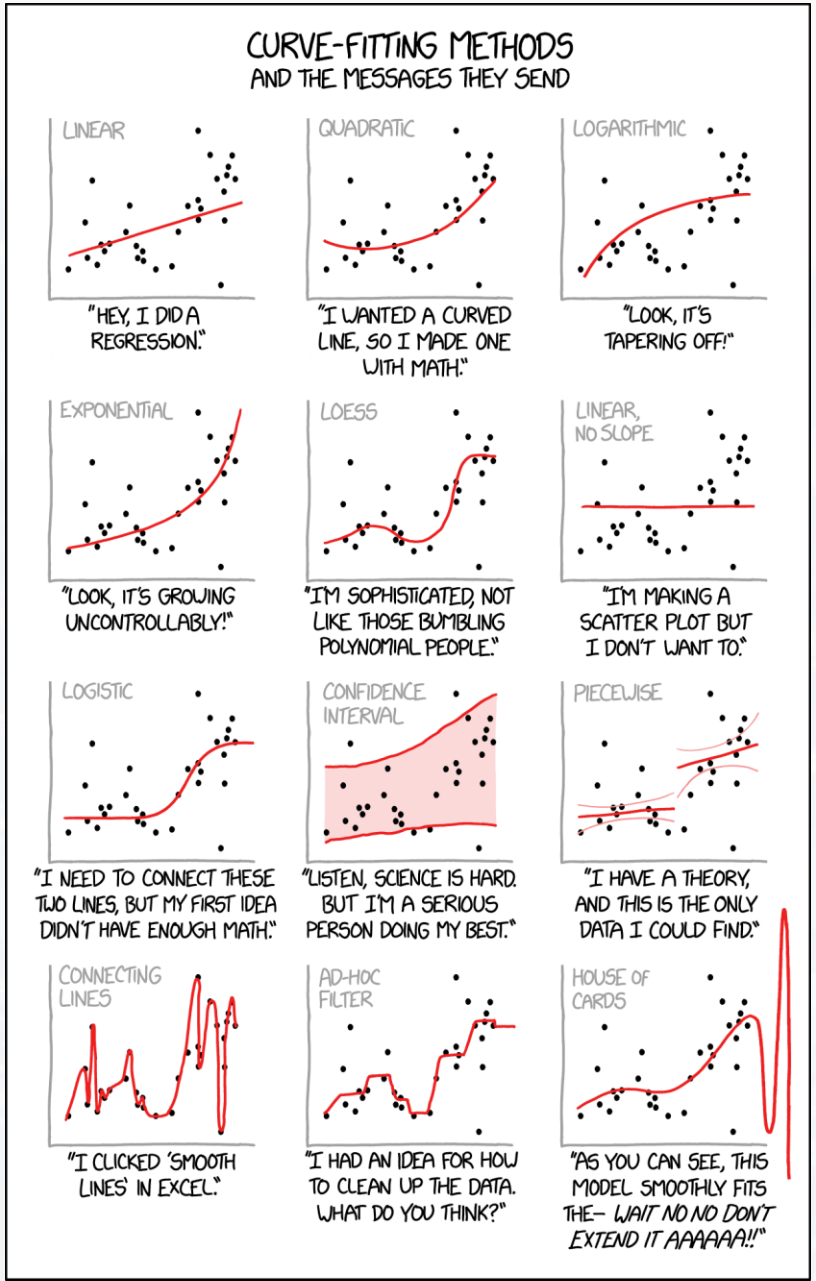
$$\hat{\varepsilon} = Y - X\hat{\beta} = Y - \hat{Y} = (I - H)Y$$

hat matrix $\mathrm{H} \coloneqq \boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T$

$$\hat{\varepsilon}^T\hat{\varepsilon} = [(I - H)Y]^T(I - H)Y = Y^T(I - H)^T(I - H)Y = Y^T(I - H)Y$$

sum of squared errors (SSE)

Maximum Likelihood Estimation, Linear Regression



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$$\hat{\beta} = \underset{\beta}{argmin}\left\{\frac{1}{N}\|Y - X\beta\|^2\right\}$$

λ *Lagrangian Multiplier*

$$\hat{\beta} = \underset{\beta}{argmin}\left\{\frac{1}{N}\|Y - X\beta\|^2 + \boldsymbol{\lambda\|\beta\|^1}\right\}$$

the Loss Function
$\boldsymbol{L(X, Y, \lambda)}$

L1 or **L**east **a**bsolute **s**hrinkage and **s**election **o**perator
- encourages **sparsity** of β
- reduces **overfitting**

$$\hat{\beta} = \underset{\beta}{argmin}\left\{\frac{1}{N}\|Y - X\beta\|^2 + \boldsymbol{\lambda\|\beta\|^2}\right\}$$

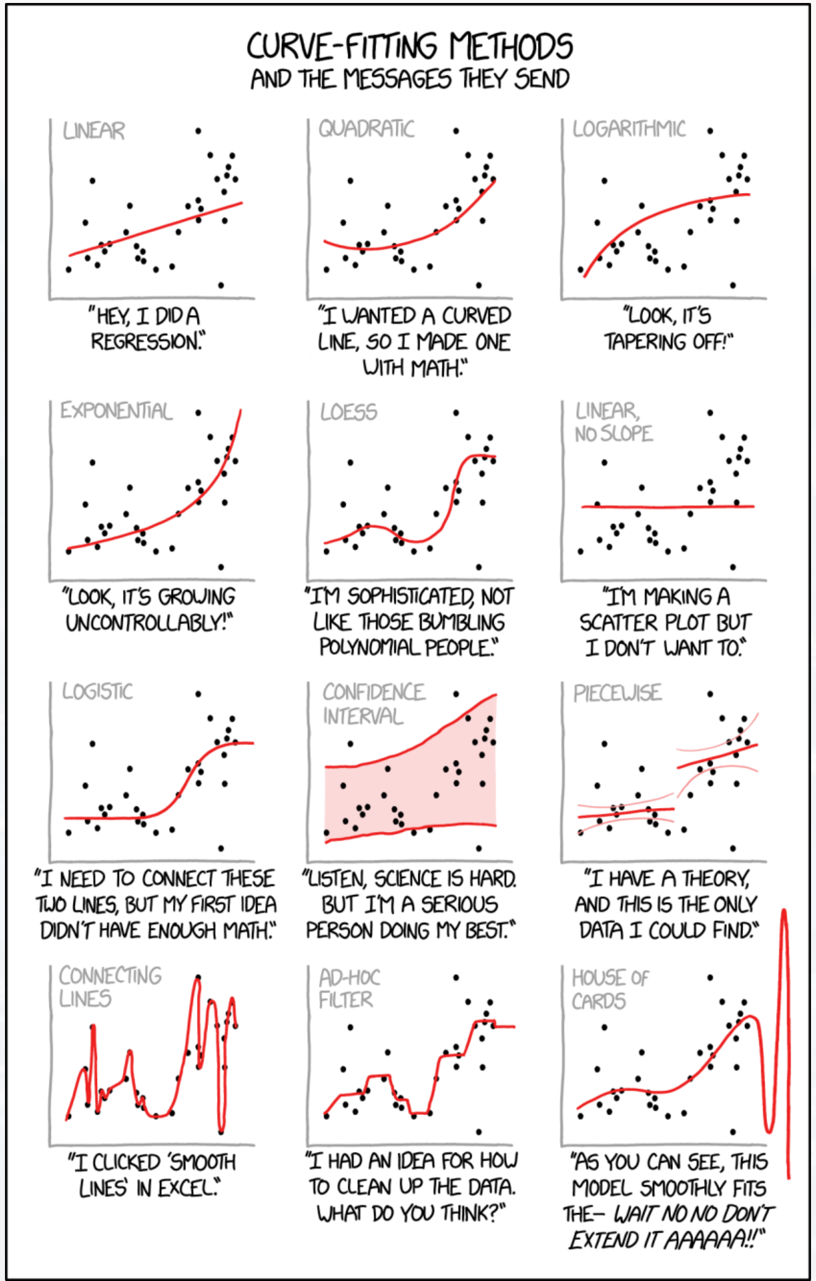
L2 or **Ridge**
- **penalizes large $\boldsymbol{\beta}$**

$$\hat{\beta} = \underset{\beta}{argmin}\left\{\frac{1}{N}\|Y - X\beta\|^2 + \boldsymbol{\lambda\, max(0, -\beta)}\right\}$$

- **penalizes negative $\boldsymbol{\beta}$**

...and so on

Maximum Likelihood Estimation, Linear Regression



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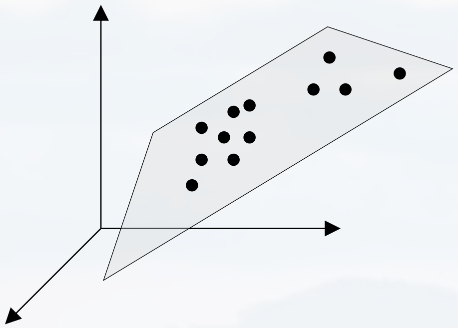
Maximum Likelihood Estimation, Linear Regression:

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon_k$$

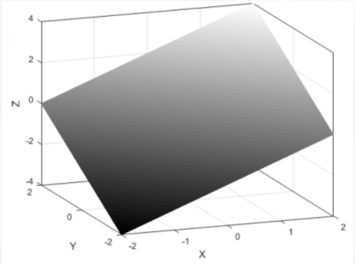
the classical model is very limiting



general: linear refers to the **factors**

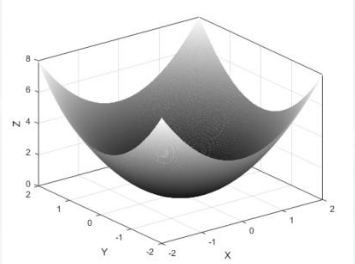
$$y_k = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

2*D* plane in 3*D* space



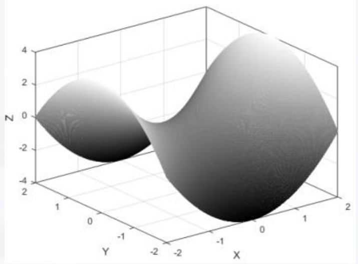
$$y_k = \beta_0 + \beta_1 {x_1}^2 + \beta_2 {x_2}^2$$

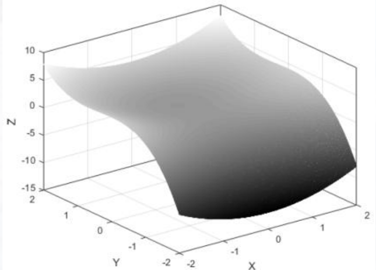
2*D* parabolic

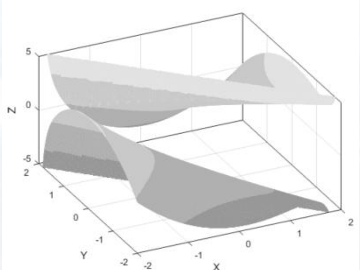


$$y_k = \beta_0 + \beta_1 {x_1}^2 - \beta_2 {x_2}^2$$

2*D* hyperbolic





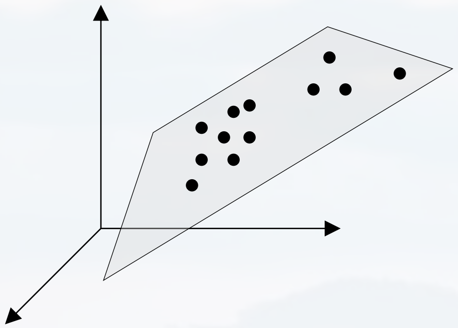


...and many more...

Maximum Likelihood Estimation, Linear Regression:

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon_k$$

the classical model is very limiting

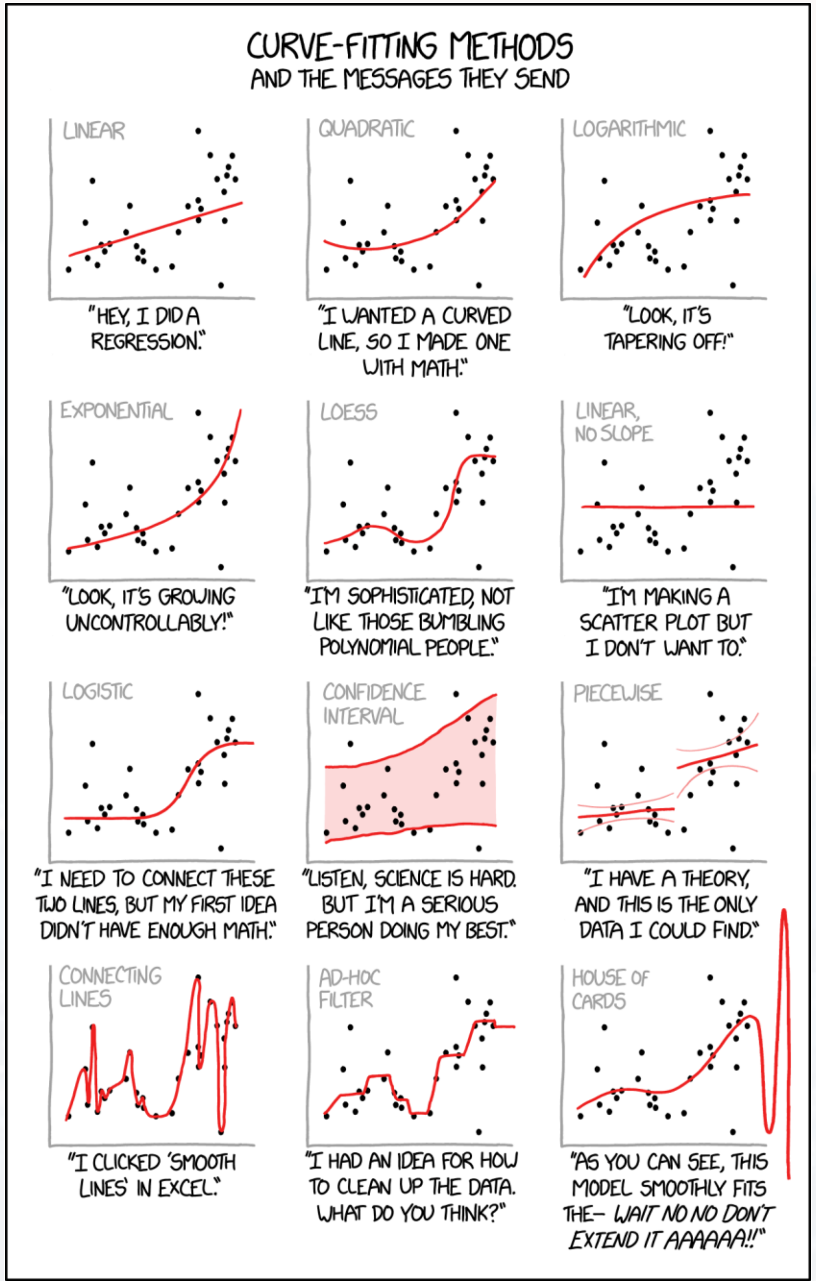


general: linear refers to the **factors**

- x_n can be subject to any **basis function** $\varphi_n(x_n)$
- the matrix X is then called **design matrix** $\phi_{i,j} = \varphi_j(x_i)$
- $\widehat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T Y \ \rightarrow (\phi^T \phi)^{-1} \phi^T Y$ is called **normal equations**
- most textbooks: rows = number of observations/samples (here K)
  columns = number of features (here N)
  → one φ_j per column j
- 1D curve fit → **one feature** x: $y_k = \beta_0 + \sum_{n=1}^{N} \beta_n \, \varphi_n(x_n) + \epsilon_k$

  polynomial fit $y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_{k,n}^n + \epsilon_k$

Maximum Likelihood Estimation, Linear Regression



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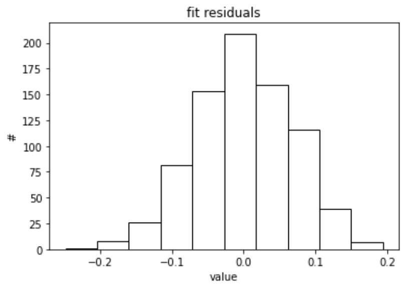
Maximum Likelihood Estimation, Linear Regression:

We now want to apply MLE to our problem and see how it leads to the same structure for $\hat{\boldsymbol{\beta}}$

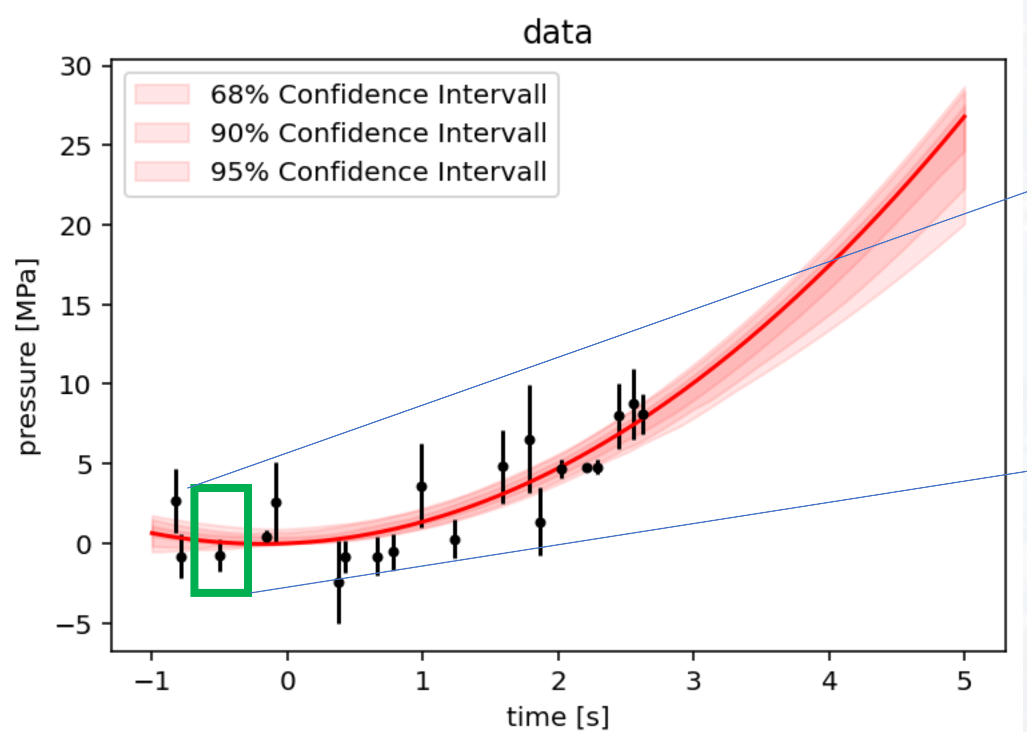
$Y = X\beta + \varepsilon$ ε: additive gaussian noise around $\mu = 0$

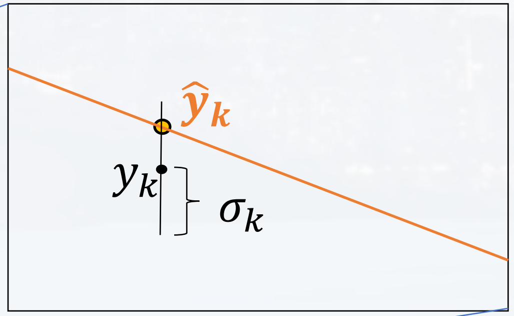


function $\boldsymbol{y(x, \beta)}$

we aim to predict a target value $\hat{\boldsymbol{y}}$

$\hat{\boldsymbol{y}} = \boldsymbol{y(x, \beta)} + \varepsilon$ for each data point *k*

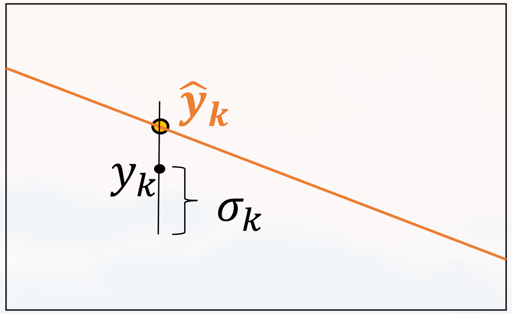




Maximum Likelihood Estimation, Linear Regression:

$$p(\hat{y}|\beta,\sigma) = \prod_{k=1}^{K} N(\hat{y}_k|\beta^T\phi(x_k),\sigma)$$

note: we assume $\sigma_k = const = \sigma$ for simplification



$$\ln[p(\hat{y}|\beta,\sigma)] = -\frac{K}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{k=1}^{K}[\hat{y}_k - \beta^T\phi(x_k)]^2$$

We want to find $\hat{\boldsymbol{\beta}}$ via MLE: gradient of $\ln[p(\hat{y}|\beta,\sigma)]$ wrt β

$$grad\{\ln[p(\hat{y}|\beta,\sigma)]\}_\beta = \frac{1}{\sigma^2}\sum_{k=1}^{K}[\hat{y}_k - \beta^T\phi(x_k)]\phi(x_k)^T$$

setting the gradient to zero: $\boxed{\hat{\boldsymbol{\beta}} = (\phi^T\phi)^{-1}\phi^T\hat{y}}$ as before

for different σ_k we find $\chi^2 = \sum_{k=1}^{K}\left(\frac{\hat{y}_k - \beta^T\phi(x_k)}{\sigma_i}\right)^2$

Thank you very much for your attention!