UNIVERSITY OF CAMBRIDGE

Advanced Data Science

Lecture 6 : Generalised Linear Models

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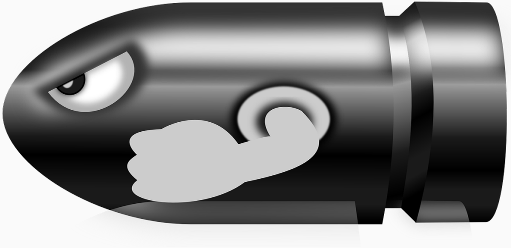
What is Machine Learning



What does Machine Learning do?

$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta)p(\theta)}{p(\mathcal{D}}$$

The Gap

Access enormous inductive bias in what data to acquire

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Assess human bias in what questions will probably be asked

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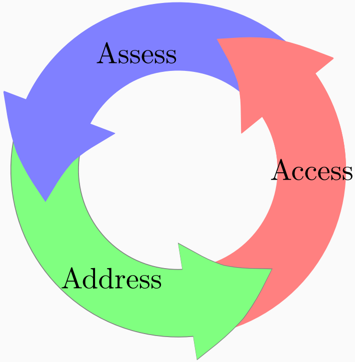
Assess human bias in what questions will probably be asked

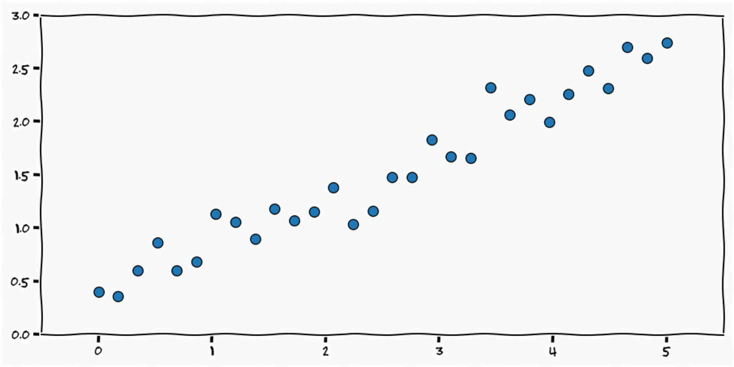
Address "it is just curve fitting"

Requirements for Data Science



Generalised Linear Models

Formalism

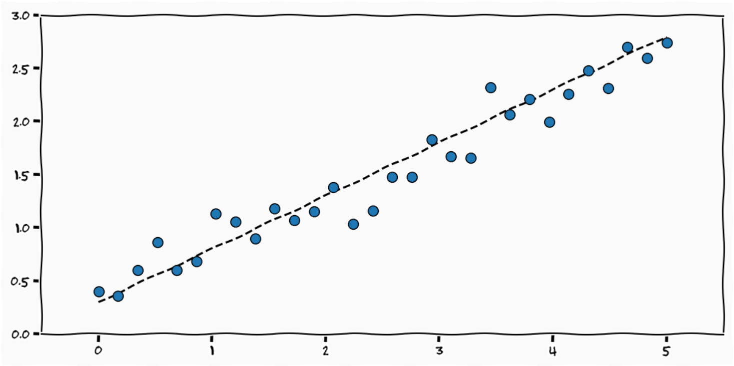


$\mathbf{x} \in \mathcal{X}$ explanatory variable

$y \in \mathcal{Y}$ response variable

Task *explain the response by the explanatory variables*

Linear Regression [Bishop, 2006]



$$y_i = \sum_{j=1}^{d} \beta_j x_{ij} + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2).$$

Linear Regression Prediction

$$\mathbb{E}[y_i \mid \mathbf{x}_i] = \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij} + \epsilon\right]$$

Linear Regression Prediction

$$
\begin{aligned}
\mathbb{E}[y_i \mid \mathbf{x}_i] &= \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij} + \epsilon\right] \\
&= \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij}\right] + \mathbb{E}[\epsilon]
\end{aligned}
$$

Linear Regression Prediction

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&= \mathbb{E}\left[\sum_{j=1}^{d} \beta_j x_{ij}\right] + \mathbb{E}[\epsilon] \\
&= \sum_{j=1}^{d} \beta_j x_{ij} + 0.
\end{aligned}
$$

Linear Regression

$$y_i = \sum_{j=1}^{d} \beta_j x_{ij} + \epsilon,$$

Linear Regression

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$$\hat{y}_i = \sum_{j=1}^{d} \beta_j x_{ij},$$

Linear Regression

$$y_i = \sum_{j=1}^{d} \beta_j x_{ij} + \epsilon,$$

$$y_i + \epsilon = \sum_{j=1}^{d} \beta_j x_{ij},$$

$$\hat{y}_i = \sum_{j=1}^{d} \beta_j x_{ij},$$

$$\hat{y}_i \sim \mathcal{N}(\hat{y}_i \mid y_i, \sigma^2) = \mathcal{N}\left(\hat{y}_i \mid \sum_{j=1}^{d} \beta_j x_{ij}, \sigma^2\right),$$

Generalised Linear Models [McCullagh et al., 1989]

$$g(\mathbb{E}[y_i \mid \mathbf{x}_i]) = \sum_{j=1}^{d} \beta_j x_{ij},$$

$g(\cdot)$ link function

$y \sim \mathcal{D}$ Exponential Dispersion Family

$\sum_{j=1}^{d} \beta_j x_{ij}$ Linear predictor

Generalised Linear Models [McCullagh et al., 1989]

$$\mathbb{E}[y_i \mid \mathbf{x}_i] = g^{-1}\left(\sum_{j=1}^{d} \beta_j x_{ij}\right),$$

- The inverse of the *link* maps the linear predictor to the first moment of the response
- Linear regression the link is identity

[1] https://towardsdatascience.com/glms-part-iii-deep-neural-networks-as-recursive-generalized-linear-URL

Generalised Linear Models [McCullagh et al., 1989]

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- The inverse of the *link* maps the linear predictor to the first moment of the response
- Linear regression the link is identity
- Looks an awful lot like a neural network[1]

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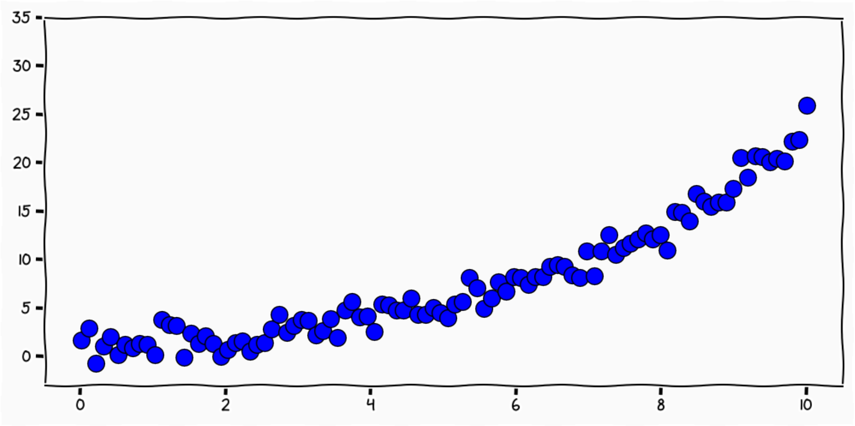
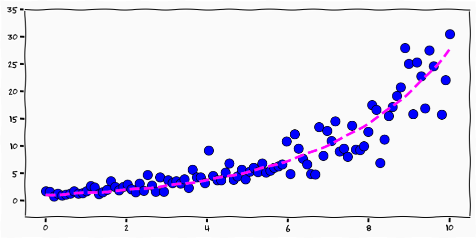
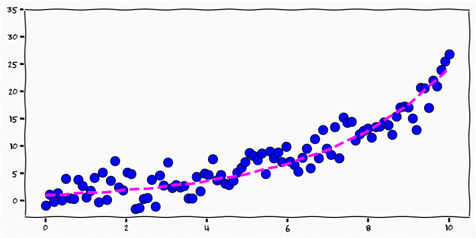


$$y_i = f(x_i) + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

Transformation vs GLM





$$\log(y_i) = \sum_{j=1}^{d} \beta_j x_{ij} + \epsilon_i$$

$$y_i = e^{\sum_{j=1}^{d} \beta_j x_{ij} + \epsilon_i} = e^{\sum_{j=1}^{d} \beta_j x_{ij}} e^{\epsilon_i}$$

$$\log(\hat{y}_i) = \sum_{j=1}^{d} \beta_j x_{ij}$$

$$y_i = e^{\sum_{j=1}^{d} \beta_j x_{ij}} + \epsilon$$

Exponential Dispersion Family [2]

$$f(y;\theta,\phi) = e^{\frac{\theta y - b(\theta)}{a(\phi)} + c(y,\phi)},$$

θ location parameter

ϕ scale parameter

i.i.d. we will assume that the data is drawn i.i.d.

[2] https://en.wikipedia.org/wiki/Exponential_dispersion_model

Gaussian

$$f(y;\mu,\sigma^2) = e^{\frac{\mu y - \frac{1}{2}\mu^2}{\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)}$$

- $\theta = \mu$
- $\phi = \sigma^2$
- $b(\theta) = \frac{1}{2}\mu^2$
- $a(\phi) = \sigma^2$
- $c(y,\phi) = \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)$

Moments

$$\mathbb{E}[y \mid \mathbf{x}] = \frac{\partial}{\partial\theta} b(\theta)$$
$$\mathbb{V}[y \mid \mathbf{x}] = a(\phi) \frac{\partial^2}{\partial\theta^2} b(\theta).$$

- Through a consistent parametrisation we can generalise the moment calculations

Statsmodels

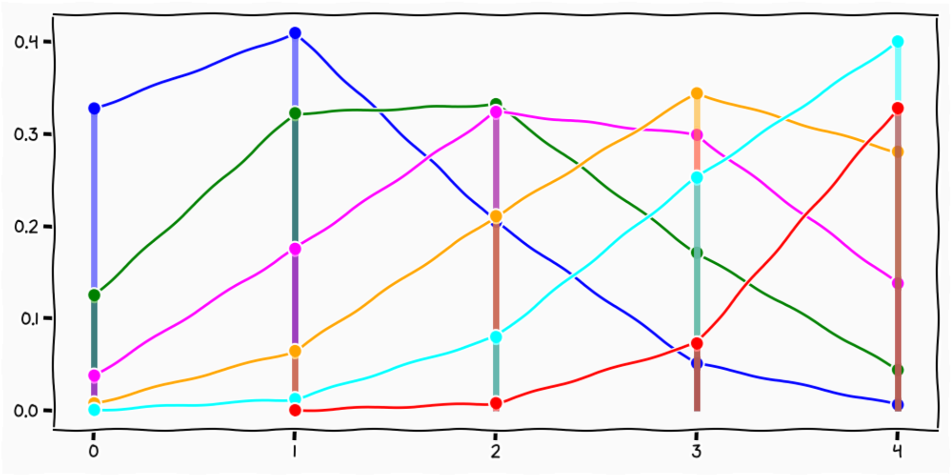
Code

```
import statsmodels.api as sm
m = sm.GLM(y, x, sm.families.Gaussian(sm.families.links.log()))
m_r = m.fit()
y_p = m_r.get_prediction(x_p).summary_frame(alpha=0.05)['mean']
```

Families `Binomial`, `Gamma`, `Gaussian`, `InverseGaussian`, `NegativeBinomial`, `Poisson`, `Tweedie`

Link Functions `CLogLog`, `LogLog`, `Log`, `Logit`, `NegativeBinomial`, `Power`, `cauchy`, `identity`, `inverse_power`, `inverse_squared`, `nbinom`, `probit`

Binomial Distribution



Binomial Regression

$$g(y_i) = \beta_0 + \beta_1 x_{i1}$$
$$y_i \sim \text{Binom}(n, p)$$

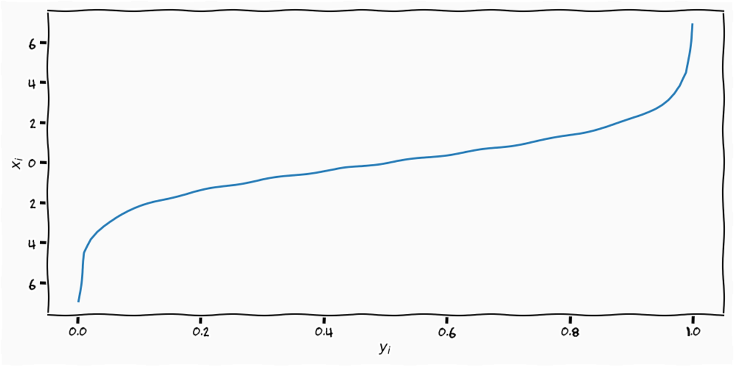
- y_i is a frequency or odds

Binomial Regression

$$g(y_i) = \beta_0 + \beta_1 x_{i1}$$
$$y_i \sim \mathrm{Binom}(n, p)$$

- y_i is a frequency or odds
- need to pick a link function that limits to $y_i \in [0, 1]$

Logit-Link



$$\mathrm{logit}(y_i) = \log\left(\frac{y_i}{1 - y_i}\right)$$

Sigmoid Function

$$\text{logit}(y_i) = \log\left(\frac{y_i}{1 - y_i}\right) = \beta_0 + \beta_1 x_{i1}$$

Sigmoid Function

$$\text{logit}(y_i) = \log\left(\frac{y_i}{1-y_i}\right) = \beta_0 + \beta_1 x_{i1}$$

$$\frac{y_i}{1-y_i} = e^{\beta_0+\beta_1 x_{i1}}$$

Sigmoid Function

$$\begin{aligned}
\operatorname{logit}(y_i) = \log\left(\frac{y_i}{1-y_i}\right) &= \beta_0 + \beta_1 x_{i1} \\
\frac{y_i}{1-y_i} &= e^{\beta_0+\beta_1 x_{i1}} \\
y_i(1+e^{\beta_0+\beta_1 x_{i1}}) &= e^{\beta_0+\beta_1 x_{i1}}
\end{aligned}$$

Sigmoid Function

$$
\begin{aligned}
\text{logit}(y_i) = \log\left(\frac{y_i}{1-y_i}\right) &= \beta_0 + \beta_1 x_{i1} \\
\frac{y_i}{1-y_i} &= e^{\beta_0+\beta_1 x_{i1}} \\
y_i(1+e^{\beta_0+\beta_1 x_{i1}}) &= e^{\beta_0+\beta_1 x_{i1}} \\
y_i &= \frac{e^{\beta_0+\beta_1 x_{i1}}}{1+e^{\beta_0+\beta_1 x_{i1}}}
\end{aligned}
$$

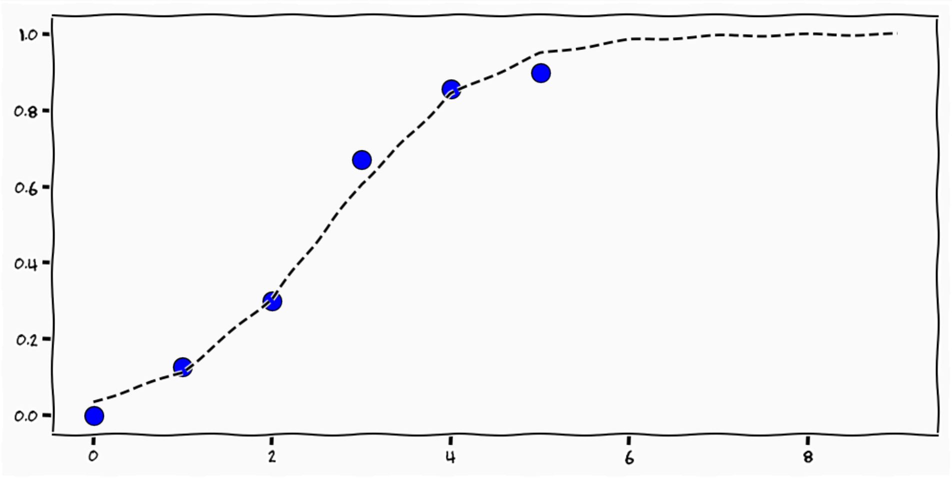
Sigmoid Function

$$
\begin{aligned}
\operatorname{logit}(y_i) = \log\left(\frac{y_i}{1-y_i}\right) &= \beta_0 + \beta_1 x_{i1} \\
\frac{y_i}{1-y_i} &= e^{\beta_0+\beta_1 x_{i1}} \\
y_i(1 + e^{\beta_0+\beta_1 x_{i1}}) &= e^{\beta_0+\beta_1 x_{i1}} \\
y_i &= \frac{e^{\beta_0+\beta_1 x_{i1}}}{1+e^{\beta_0+\beta_1 x_{i1}}} \\
&= \frac{1}{1+e^{-(\beta_0+\beta_1 x_{i1})}}
\end{aligned}
$$

Binomial Data [Weisberg, 2005]

Current	Trials	Response	Proportion
0	70	0	0.00
1	70	9	0.129
2	70	21	0.300
3	70	47	0.671
4	70	60	0.857
5	70	63	0.900

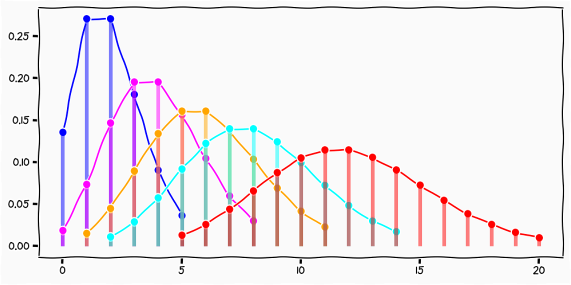
Logistic Regression



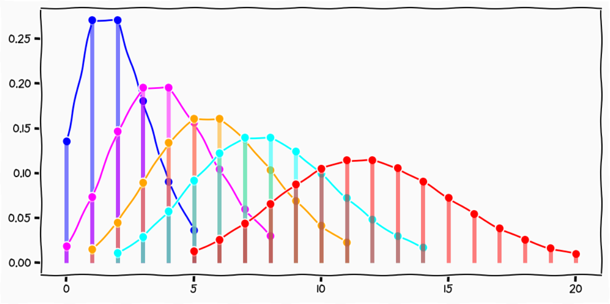

```
sm.GLM(y, X, sm.families.Binomial(sm.families.links.logit()))
```

Poisson Distribution

- Arrival times
- Website visitors
- Job cue for server
- Failures of product



Poisson Distribution



$$\text{Poisson}(y_i) = \frac{e^{-\lambda}\lambda^y}{y!}$$

$$\mathbb{E}[y_i] = \lambda$$

Poisson Regression

- Counts are positive so we need a positive link function

$$\log(\lambda_i) = \sum_{j=1}^{d} \beta_j x_{ij}$$

Poisson Regression

- Counts are positive so we need a positive link function

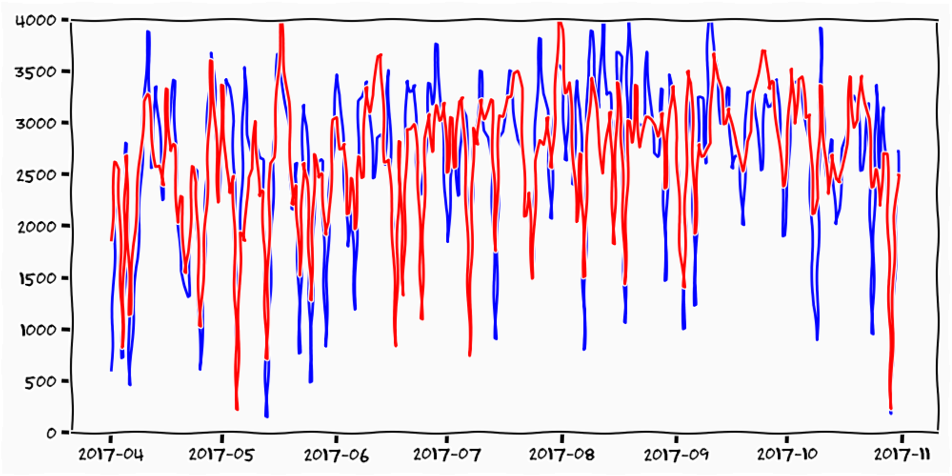
$$\log(\lambda_i) = \sum_{j=1}^{d} \beta_j x_{ij}$$

- Leads to the following model

$$p(y_i \mid x_i) = \frac{e^{-\lambda_i} \lambda_i^{y}{}_i}{y_i!} = \frac{e^{-\left(e^{\sum_{j=1}^{d} \beta_j x_{ij}}\right)} \left(e^{\sum_{j=1}^{d} \beta_j x_{ij}}\right)^{y_i}}{y_i!}$$

Day	Day of Week	Month	High Temp	Low Temp	Percipitation	Cyclists
1.0	5.0	4.0	46.0	37.0	0.00	606.0
2.0	6.0	4.0	62.1	41.0	0.00	2021.0
3.0	0.0	4.0	63.0	50.0	0.03	2470.0
4.0	1.0	4.0	51.1	46.0	1.18	723.0
6.0	3.0	4.0	48.9	41.0	0.73	461.0
...	...	...	...	...	...	...
1	31	10	54	44	0.00	2727

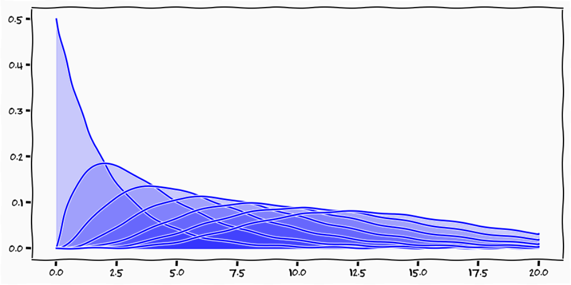
Poisson Regression




```
sm.GLM(y, X, family=sm.families.Poisson()).fit()
```

Gamma Distribution

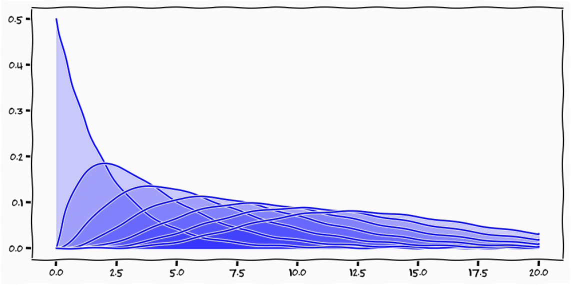
- Waiting times for Poisson events
- Variance and mean connected



Gamma Distribution

$$\text{Gamma}(y_i) = \frac{1}{\Gamma(\phi)\theta^{\phi}} y_i^{\phi-1} e^{-\frac{y_i}{\theta}}$$

$$\mathbb{E}[y_i] = \phi\theta$$
$$\mathbb{V}[y_i] = \phi\theta^2$$



Gamma Regression

- Exponential Dispersion Gamma

$$\text{Gamma}(y_i) = e^{\frac{y_i\theta_i - \log\left(-\frac{1}{\theta_i}\right)}{\phi} + \frac{1-\phi}{\phi}\log(y_i) - \log\left(\Gamma(\phi^{-1})\right)}$$

Gamma Regression

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- If you "derive" the canonical link function from the distribution it should be,

$$-\frac{1}{\theta} = \sum_{j=1}^{d} \beta_j x_{ij}$$

Gamma Regression

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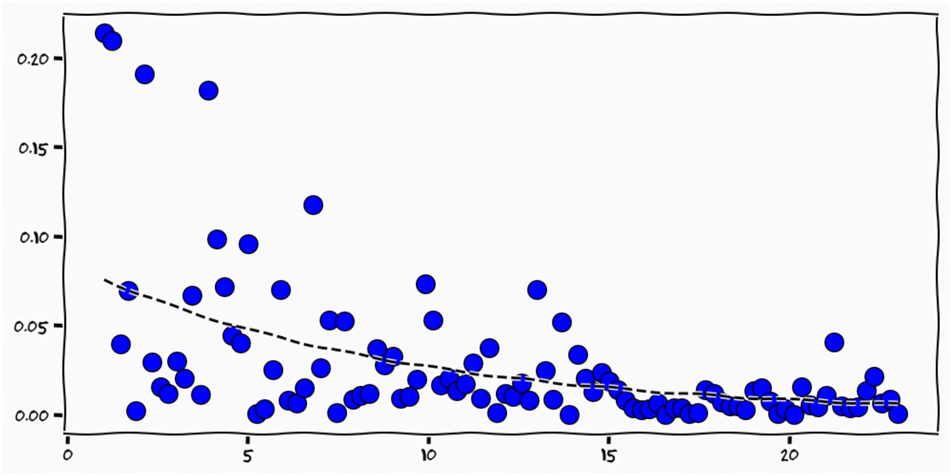
- If you "derive" the canonical link function from the distribution it should be,

$$-\frac{1}{\theta} = \sum_{j=1}^{d} \beta_j x_{ij}$$

- Gamma regression is most commonly used with `log` as the link

$$\log(\mathbb{E}[y_i \mid \mathbf{x}_i]) = \sum_{j=1}^{d} \beta_j x_{ij}$$

Gamma Regression



Model	Response Variable	Link	Explanatory Variable
Linear Regression	Normal	Identity	Continuous
Logistic Regression	Binomial	Logit	Mixed
Poisson Regression	Poisson	Log	Mixed
ANOVA	Normal	Identity	Categorical
ANCOVA	Normal	Identity	Mixed
Loglinear	Poisson	Log	Categorical
Multinomial response	Multinomial	Generalized Logit	Mixed

Inference

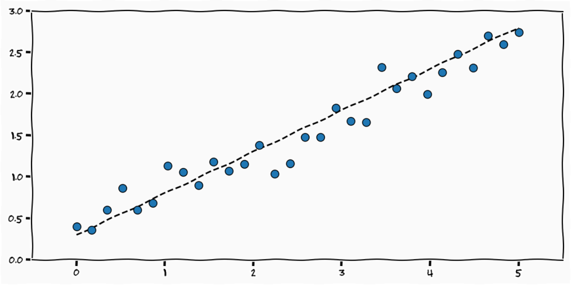
$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmax}} \prod_{i=1}^{N} p(y_i \mid \boldsymbol{\beta}, \mathbf{x}_i)$$

- In general gradient descent on `log-likelihood`
- For specific models there are tailored inference schemes

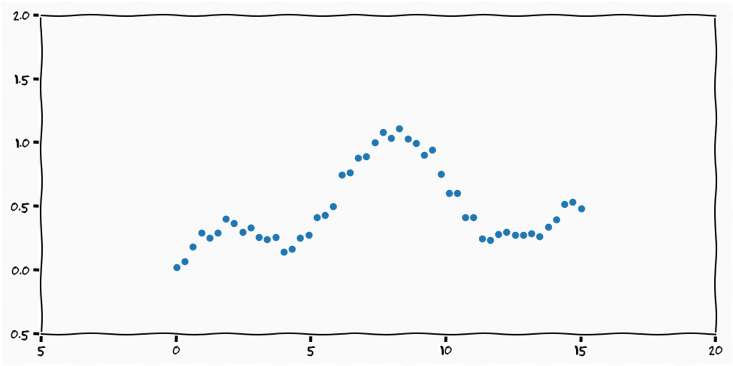
Design Matrix

Design Matrix

$$\mathbf{X} = \begin{bmatrix} x_0 & 1 \\ x_1 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{bmatrix}$$



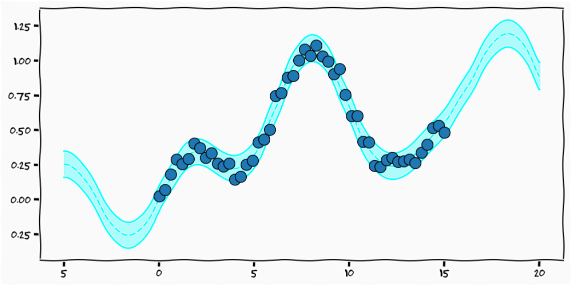
Non-Linear Function



$$y = 0.2\sin(x) + \sin\left(\frac{x^2}{40}\right) + 0.05x$$

Design Matrix

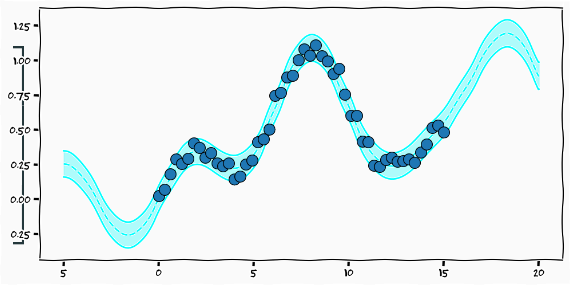
$$\mathbf{X} = \begin{bmatrix} \sin(x_0) & \sin(\frac{x_0^2}{40}) & x_0 \\ \sin(x_1) & \sin(\frac{x_1^2}{40}) & x_1 \\ \vdots & \vdots & \vdots \\ \sin(x_N) & \sin(\frac{x_N^2}{40}) & x_N \end{bmatrix}$$



$$\boldsymbol{\beta} = [0.2155, 0.4956, 0.0482]$$

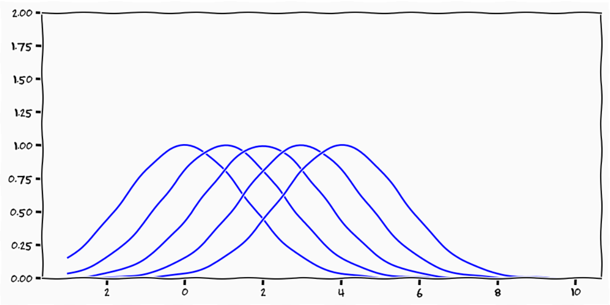
Over-parametrised matrix

$$\begin{bmatrix} \sin(x_0) & \sin(\frac{x_0^2}{40}) & x_0 & -\sin(x_0) \\ \sin(x_1) & \sin(\frac{x_1^2}{40}) & x_1 & -\sin(x_1) \\ \vdots & \vdots & \vdots & \vdots \\ \sin(x_N) & \sin(\frac{x_N^2}{40}) & x_N & -\sin(x_N) \end{bmatrix}$$



$$\boldsymbol{\beta} = [0.1078, 0.4956, 0.0482, 0.1078]$$

Localised Basis Function



$$g\left(\mathbb{E}[y_i \mid \mathbf{x}_i]\right) = \sum_{j=1}^{N} \beta_j \phi(\mathbf{x}_j, \mathbf{x}_i), \qquad \phi(\mathbf{x}_j, \mathbf{x}_i) = e^{-\frac{(\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}}(\mathbf{x}_i - \mathbf{x}_j)}{\ell^2}}$$

Regularisation

Solution bias

$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmax}} \prod_{i=1}^{N} p(y_i \mid \boldsymbol{\beta}, \mathbf{x}_i)$$

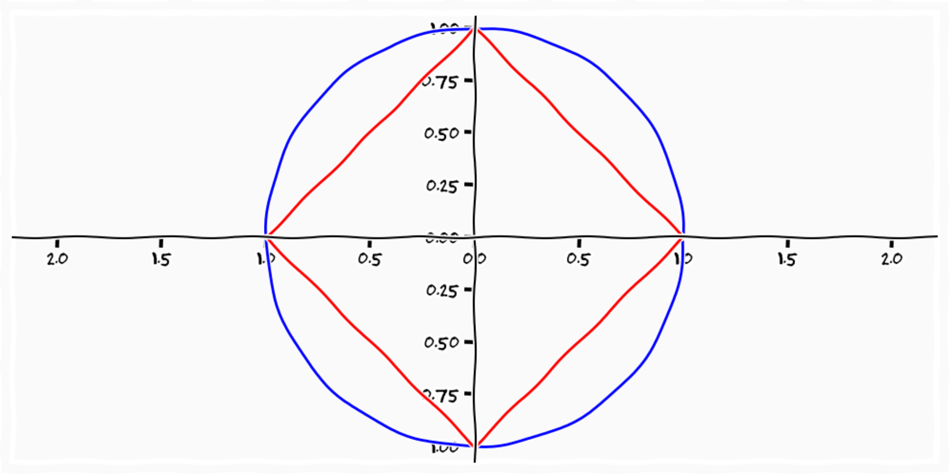
- Maximum Likelihood encodes no preference towards any solution
- Due to optimisation procedure we might get very different results

Norm

$$\hat{\boldsymbol{\beta}} = \operatorname*{argmax}_{\boldsymbol{\beta}} \prod_{i=1}^{N} p(y_i \mid \boldsymbol{\beta}, \mathbf{x}_i) + \lambda \left(\sum_{j=1}^{d} \beta_j^p \right)^{\frac{1}{p}}$$

- Introduce inductive bias towards specific solutions
- Normally done using a norm

Ridge vs Lasso



Code

```
m.fit_regularized(alpha=0.10,L1_wt=0.0)
```

- `L1_wt` 0 → `Ridge`, 1 → `Lasso`
- `alpha` the penalty

Summary

Response Variable Distribution How is your response variable distributed?

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Link Function How is the scale parameter of the distribution related to the explanatory variables

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Link Function How is the scale parameter of the distribution related to the explanatory variables

Design Matrix What is the features of the explanatory variables?

Response Variable Distribution How is your response variable distributed?

Link Function How is the scale parameter of the distribution related to the explanatory variables

Design Matrix What is the features of the explanatory variables?

Regulariser What is the "preferred" solution?

Thoughts

- Can you split up the data by some criterion?

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    - localised GLM

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- Can you remove the effect of one model from data and then retrain on residual?

Thoughts

- Can you split up the data by some criterion?
  - localised GLM
- Can you remove the effect of one model from data and then retrain on residual?
- You will not be able to find the "perfect" model, but show that you can reason about these models!!

eof

References

Bishop, Christopher M. (2006). *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Secaucus, NJ, USA: Springer-Verlag New York, Inc.

McCullagh, P. and J. A. Nelder (1989). *Generalized Linear Models*. London, UK: Chapman Hall / CRC: Chapman Hall / CRC.

Weisberg, Sanford (2005). *Applied Linear Regression*. Wiley Series in Probability and Statistics. John Wiley & Sons, Inc., nil.