### GLMs and Causal Inference

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GLM examples

Causal Inference

### GLM Interlude



- Some more GLM examples...
- Before looking at details for non-parametrics, let us re-visit the details of the GLM specification.
- Recall for a Bernoulli random variable has pmf

$$f_Y(y) = \theta^y \{1 - \theta\}^{1 - y}$$

$$= \exp\{y \log \frac{\theta}{1 - \theta} + \log(1 - \theta)\}. \tag{1}$$

Clearly here we set  $\phi = \log \frac{\theta}{1-\theta}$ . We can solve for  $\exp(\phi) = \frac{\theta}{1-\theta}$ , with

$$heta = rac{1}{1 + \exp(\phi)} \Rightarrow 1 - heta = rac{\exp(\phi)}{1 + \exp(\phi)}.$$

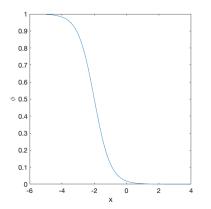
For example we could look at a single covariate  $x_i$  and set

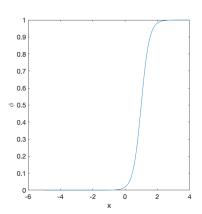
$$\phi_i = \beta_0 + \beta_1 x_i.$$

We see directly that as  $\phi$  ranges across any value,  $\theta$  is constrained to lie between zero and unity.

## **GLM** Interlude







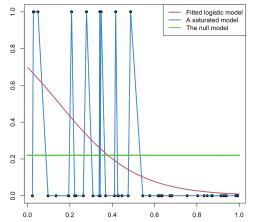
### GLM Interlude



• We can examine the improvement using the deviance. Recall that

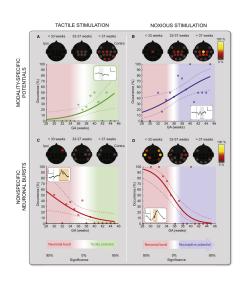
$$D = 2\{\ell_n(\widehat{\phi}) - \ell_n(\widehat{\beta})\}.$$

So we can fit both models and compare



### Bernoulli and Binomial





### Poisson observations



Looking at the Poisson pmf we have

$$f_Y(y) = \frac{e^{-\mu} \mu^y}{y!} = \exp\{-\mu + y \log(\mu) - \ln y!\}.$$
 (2)

Here we clearly set  $\phi = \log(\mu)$ . Solving for  $\mu$  just gives us  $\mu = \exp(\phi)$ . We only need the mean to remain positive so this will fix our problem.

• Again we use the deviance to assess the fit; and would compare to the model  $\mu_i$  is different for each value of i.

## What about the sparse GLM?



• Hastie and Park (2007) estimate the parameters of the GLM using

$$\hat{\beta}_{\mathit{L}}(\lambda) = \arg\min_{\beta} \{ -\log \mathit{L}(\beta) + \lambda \|\beta\|_{1}. \} \quad \text{a version of LASSO generalized for GLMs}$$

- This mimics using the Lasso for the Gaussian linear model.
- We can study the geometry of this space in β. <u>Unfortunately unlike</u> the LASSO it is not a convex optimisation problem. This means we are not seeing the possibility of a polynomial-time algorithm solving our problem. We could also end up with multiple optima.
- Hastie and Park also extended the elastic net to this setting

$$\hat{\beta}_{EN}(\lambda_1, \lambda_2) = \arg\min_{\beta} \left\{ -\log L(\beta) + \lambda_1 \|\beta\|_1 + \lambda_2 \|\beta\|_2^2 \right\}. \tag{3}$$

• This has two penalties. Problems that arise when X has linearly dependent columns; the coefficient estimates are highly unstable.

## What about the sparse GLM?



- When  $\lambda_2$  is a constant, and  $\lambda_1$  varies in an open set, such that the current active set remains the same, a unique, continuous and differentiable function.
- The additional penalization of the elastic net, is not either yielding a convex problem.
- Just optimizing the GLM likelihood can be problematic on its own.
- This brings us back to the penalized GLM. Augugliaro et al (2013) looked at the differential geometry of this problem.

## GLM Nonparametric relationships with $x_i$



So far: how to estimate  $g:\mathbb{R}\to\mathbb{R}$  (assumed smooth) in

$$Y_i = g(x_i) + arepsilon_i, \quad arepsilon_i \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2), ext{ given data } \quad \{(Y_i, x_i)\}_{i=1}^n.$$

Can extend to GLM setting as:

$$|Y_i|x_i \stackrel{indep}{\sim} \exp\left\{g(x_i)y - \gamma(g(x_i)) + S(y)\right\}$$

ullet Parametrise candidate g via spline

a spline 
$$s(x) = \sum_{j=1}^{n} \gamma_{j} B_{j}(x).$$
 Some  $y$  as purious lecture

• Define matrices B and  $\Omega$  as before,

$$B_{ij}=B_j(x_i), \quad \Omega_{ij}=\int B_i''(x)B_j''(x)dx$$

And consider penalised likelihood, similarly as with penalised GLM

Define matrices 
$$B$$
 and  $\Omega$  as before, 
$$B_{ij} = B_j(x_i), \quad \Omega_{ij} = \int B_i''(x)B_j''(x)dx$$
And consider penalised likelihood, similarly as with penalised GLM 
$$\ell_n(\gamma) + \lambda \gamma^\top \Omega \gamma = \gamma^\top B^\top Y - \sum_{i=1}^n \gamma(b_i^\top \gamma) + \lambda \gamma^\top \Omega \gamma.$$
Risky Risky Regulator



### How can we generalise to multivariate covariates?

lacktriangle "Immediate" Generalisation:  $g:\mathbb{R}^p o\mathbb{R}$  (smooth)

$$Y_j = g(x_{j1}, \ldots, x_{jp}) + arepsilon_j, \quad arepsilon_j \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2)$$

- ▶ Estimation by (e.g.) multivariate kernel method.
- ▶ Two basic drawbacks of this approach . . .
- Shape of kernel? (definition of local)





## GLM Nonparametric relationships with $x_i$

#### What is "local" in $\mathbb{R}^p$ , though?

- → Need some definition of "local" in the space of covariates
- $\hookrightarrow$  Use some metric on  $\mathbb{R}^p \ni (x_1, \dots, x_p)^\top$ !

#### But which one?

- Choice of metric choice of geometry
  - ← e.g., curvature reflects intertwining of dimensions
- Geometry  $\implies$  reflects structure in the covariates
  - potentially different units of measurement (variable stretching of space)
  - a may be of higher variation in some dimensions (need finer neighbourhoods there)
  - statistical dependencies present in the covariates ("local" should reflect these)



## GLM Nonparametric relationships with $x_i$

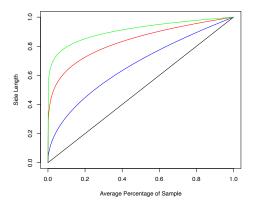


Figure: Curse of Dimensionality (Unif[0, 1] $^p$ ): p = 1, p = 2, p = 5, p = 10





### Curse of Dimensionality

"neighbourhoods with a fixed number of points become less local as the dimensions increase"

Bellman (1961)

- Hence to allow for reasonably small bandwidths
   → Density of sampling must increase.
- → Density of sampling must increase
- Need to have ever larger samples as dimension grows.



Attempt to find a link/compromise between:

- our mastery of 1D case (at least we can do that well . . . ),
- and higher dimensional covariates (and associated difficulties).

Additive models: proposed to get around curse of dimensionality: it captures variation in one variable, but allows for difference functions for each variable.

Perhaps something that can be fitted/interpreted variable-by-variable?

 $Y_i = \alpha_i + \sum_{k=1}^p f_k(x_{ik}) + \varepsilon_i, \quad \varepsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2),$ 

with  $f_k$ 's univariate smooth functions,  $\sum_i f_k(x_{ik}) = 0$ .

if we have random vars which are no longer Gaussian

► Can extend to Generalised Additive Model:

$$|Y_i|x_i^{ op} \stackrel{indep}{\sim} \exp\left\{lpha_i y + y \sum_{k=1}^p rac{f_k}{f_k}(x_{ik}) - \gamma\left(lpha_i + \sum_{k=1}^p f_k(x_{ik})
ight) + S(y)
ight\}$$



- ▶ How to fit additive model? Consider Gaussian case only for simplicity.
- $\hookrightarrow$  Know how to fit each  $f_k$  separately quite well
- ► Consider *i*th response:

$$\mathbb{E}\left[Y_i - \alpha - \sum_{m \neq k} f_m(x_{im})\right] = f_k(x_{ik})$$

- ► Suggests the Backfitting Algorithm:
- (1) Initialise:  $\alpha = \overline{Y}$ ,  $f_k = f_k^0$ ,  $k = 1, \dots, p$ .
- (2) Cycle: Get  $f_k$  by 1D smoothing of partial residual scatterplot

$$\left\{\left(Y_i-lpha-\sum_{m
eq k}f_m(x_{im}),x_{ik}
ight)
ight\}_{i=1}^n=\{e_{ik},x_{ik}\}_{i=1}^n.$$

- (3) Stop: when individual functions don't change
- ► Any smoother can be used, usually splines. (cc KOEs)



A different approach is inspired by tomography. Model Gaussian response as:

$$Y_i = \underbrace{\sum_{k=1}^K h_k(x_i^ op eta_k)}_{=g(x_i^ op)} + arepsilon_i, \quad ||eta_k|| = 1, \,\, arepsilon_i \,\, \overset{ ext{i.i.d.}}{\sim} \,\, \mathcal{N}(0,\sigma^2).$$

- Also additively decomposes g into smooth functions  $h_k : \mathbb{R} \to \mathbb{R}$ .
- ullet But each function now depends on a global linear feature  $oldsymbol{x}_i^ opoldsymbol{eta}_k$ 
  - $\hookrightarrow$  a linear combination of the covariates
  - $\hookrightarrow ||\beta_k|| = 1$  for identifiability.
- Projections directions to be chosen for best fit (nonlinear problem)
- Each  $h_k$  is a ridge function of  $x_i^{\top}$ : varies only in the direction defined by  $\beta_k$

#### Pros and Cons:

- (+) By classical Fourier series, can show that any  $C^1([0,1]^p) \to \mathbb{R}$  function is uniformly approximated arbitrarily well as  $K \to \infty$ . Useful for prediction.
- (-) Interpretability? What do terms mean within problem?



#### How is the model fitted to data?

Assume only one term, K = 1 and consider penalized likelihood:

$$\min_{h_1 \in C^2[[0,1],||\beta||=1} \qquad \left\{ \sum_{i=1}^n \{Y_i - h_1(\boldsymbol{x}_i^\top \boldsymbol{\beta})\}^2 + \int_0^1 \{h_1''(t)\}^2 dt \right\}.$$

#### Two steps:

- Smooth: Given a direction eta, fitting  $h_1(x_i^{ op}eta)$  is done via 1D smoothing.
- Pursue: Given  $h_1$ , have a non-linear regression problem w.r.t.  $\beta$ .

#### Hence, iterate between the two steps

- $\hookrightarrow$  Complication is that  $h_1$  not explicitly known, so need numerical derivatives.
- → Computationally intensive (impractical in the '80's but doable today).

Further terms added in forward stepwise manner.



If  $\beta_k$  needs to be estimated non-linearly anyway...

$$g(x_i^ op) pprox \sum_{k=1}^K h_k(x_i^ op oldsymbol{eta_k})$$

Signoide\
... do we really need to estimate the  $h_k$  or can we fix them?

### Theorem (Nonlinear Sigmoidal Approximation)

Let  $\Psi: \mathbb{R} \to [0,1]$  be a strictly increasing distribution function and  $g: [0,1]^p \to \mathbb{R}$  be an arbitrary continuous function. Then, for any  $\epsilon > 0$ , there exists  $K < \infty$  and vectors  $\alpha, t \in \mathbb{R}^K$  and  $\{\beta_1, ..., \beta_K\} \subset \mathbb{R}^p$  such that

 $\begin{array}{l} \text{vectors } \alpha, t \in \mathbb{R}^{N} \text{ and } \{\beta_{1},...,\beta_{K}\} \subset \mathbb{R}^{p} \text{ such that} \\ y = \phi\left(\sum_{k=1}^{K} \alpha_{k} x^{T} y\right) \\ = \phi(x) \otimes \psi\left(\sum_{k=1}^{K} \alpha_{k} y\right)$ 

- Can take  $h_k$  to be translations of the same known function  $\Psi!$
- The tradeoff is that K may need to be quite large (interpretability?)
- Called a (single layer) neural network by analogy to synaptic function.
- A parametric model with many parameters fit by nonlinear least squares (gradient descent)



What about including transformations of the original covariates?

① Can of course include J transformations  $w_i: \mathbb{R}^p \to \mathbb{R}$ 

$$(u_1,...,u_p)\mapsto w_j(u_1,...,u_n), \qquad j=1,...,J,$$

of the original variables as additional covariates by suitably enlarging the design matrix  $\boldsymbol{X}$ .

② We simply adjoin to X another J columns of dimension  $n \times 1$  each:

$$\left(egin{array}{c} w_j(oldsymbol{x}_1^ op) \ dots \ w_j(oldsymbol{x}_n^ op) \end{array}
ight) \qquad j=1,...,J.$$

3 Which functions  $w_i$  should we pick though?

Since we've gone nonlinear anyway,

why not attempt to learn which transformations to include from the data?

# GLM Nonparametric relationships with $x_i$



#### How?

- Instead of including our original covariates (p columns of X)...
- $\circ$  ... use q derived covariates (q can be larger than p)

$$\left(egin{array}{c} w_1(x_1^ op) \ dots \ w_1(x_n^ op) \end{array}
ight), \left(egin{array}{c} w_2(x_1^ op) \ dots \ w_2(x_n^ op) \end{array}
ight), \quad \cdots \quad , \left(egin{array}{c} w_q(x_1^ op) \ dots \ w_q(x_n^ op) \end{array}
ight)$$

ullet ... where the q transformations  $\{w_j\}_{j=1}^q$  are to be estimated from the data.

Recycling our nonlinear approximation theorem, write

$$w_j(x^ op)pprox \sum_{m=1}^{M_j} \delta_{m,j} \Psi(s_{m,j}+x^ op \gamma_{m,j})$$

using the same  $\Psi$ , and needing to estimate  $(\delta_j, s_j, \gamma_{1,j}, ..., \gamma_{M_j,j})$ , for j=1,...,q.



Assuming that we've constructed our new variables, we have a new design matrix

$$\left(egin{array}{ccc} w_1(x_1^ op) & \dots & w_q(x_1^ op) \ dots & & dots \ w_1(x_n^ op) & \dots & w_q(x_n^ op) \end{array}
ight)$$

Summarising, we have defined a hierarchical nonlinear regression model:

$$Y_i = \sum_{k=1}^K lpha_k \Psi \Big( t_k + (w_i(x_1^ op),...,w_i(x_n^ op))eta_k \Big) + arepsilon_i =$$

$$egin{aligned} &= \sum_{k=1}^K lpha_k \Psi\left(\mathit{t}_k + \left(\sum_{m=1}^{M_1} \delta_{m,1} \Psi(s_{m,1} + x^ op \gamma_{m,1}), ..., \sum_{l=1}^{M_q} \delta_{l,q} \Psi(s_{l,q} + x^ op \gamma_{l,q})
ight) eta_k 
ight) + arepsilon_i \end{aligned}$$

- ... known these days as a two-layer neural network.
  - Can add more layers ("deep neural network").
  - Highly non-linear and non-convex cascade of simple nonlinearities applied to linear transformations.
  - More easily perceived visually through a graphical representation

### Causal Inference



- If we say "X causes Y"; mathematically this means *changing* the value of x *changes* the distribution of Y.
- When X causes Y then X and Y will be associated (one type of association is correlation), but the converse is generally not true.
- We shall discuss this in terms of <u>counterfactual</u> random variables.
- Let us start by a simple binary setup. Let X=1 denote the event that a unit was "treated" and X=0 denote the event that a unit was not "treated".
- We use the term "treated" in a very broad sense. Instead we might have used "exposed" and "not-exposed".
- Let *Y* be some <u>outcome variable</u>. To distinguish between association and causation we need to enhance our vocabulary.

### Causal Inference II



- Two new symbols  $C_0$  and  $C_1$  are introduced to denote potential outcomes.
- $C_0$  is the outcome if the unit was not treated, and similarly,  $C_1$  is the outcome if the unit was treated. These are both random variables. Thus

$$Y=C_X. (4)$$

This is the consistency relationship.

- Note that many things are unobserved in this model. When X=1 then we do not observe  $C_0$  for those cases; also when X=0 we do not observe  $C_1$ . We call those outcomes counterfactual.
- Thus  $(C_0, C_1)$  are hidden or latent variables.

### Causal Inference III



• Define the average causal effect to be

$$\theta = \mathbb{E}\{C_1\} - \mathbb{E}\{C_0\}. \tag{5}$$

 $\theta$  is the difference in effect if everyone was treated versus if everyone was not. If  $C_0$  and  $C_1$  were binary then we can define the causal odds ratio

$$\frac{\frac{\Pr\{C_1=1\}}{\Pr\{C_1=0\}}}{\frac{\Pr\{C_0=1\}}{\Pr\{C_0=0\}}}.$$

We also define the <u>causal relative risk</u>:

$$\frac{\Pr\{C_1 = 1\}}{\Pr\{C_0 = 1\}}.$$

• Define the association of Y with X to be

$$\alpha = \mathbb{E}\{Y \mid X = 1\} - \mathbb{E}\{Y \mid X = 0\}. \tag{6}$$

### Causal Inference III



- Theorem (Association is not causation): In general  $\theta \neq \alpha$ .
- Example: Suppose that we have observed the following units for a treatment:

Table: Causation vs association.

Χ	Y	$C_0$	$C_1$	14 × 60 m mm
0	0	0	0* ′	observe CL
0	0	0	0*	
0	0 0	0	0*	
0	0	0	0*	- if it is I we heren
1	1	1* ~	1	observe Co
1	1	1*	1	
1	_	1*	1	
1	1	1*	1	

Asterisks are indicating unobserved values.

## Causal Inference IV



• For every experimental unit  $C_0 = C_1$  and so the "treatment" has no effect.

$$\theta = \mathbb{E}\{C_1\} - \mathbb{E}\{C_0\} \tag{7}$$

$$= \frac{1}{8} \sum_{i=1}^{8} C_{1i} - \frac{1}{8} \sum_{i=1}^{8} C_{0i} = \frac{1}{8} \sum \{C_{1i} - C_{0i}\} = 0$$
 (8)

Thus the average causal effect is zero.

• We can also estimate the association:

$$\alpha = \mathbb{E}\{Y \mid X = 1\} - \mathbb{E}\{Y \mid X = 0\} = \frac{1 + 1 + 1 + 1}{4} - \frac{0 + 0 + 0 + 0}{4}$$
$$= 1.$$

Thus in this example  $\theta \neq \alpha$ .