## Econometrics: Learning from ‘Statistical Learning’ Techniques

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## Agenda

"the numbers have no way of speaking for themselves. We speak for them. [‥] Before we demand more of our data, we need to demand more of ourselves " from Silver (2012).

- (big) data
- econometrics \& probabilistic modeling
- algorithmics \& statistical learning
- different perspectives on classification
- boostrapping, PCA \& variable section see Berk (2008), Hastie, Tibshirani \& Friedman (2009), but also Breiman (2001)


## Statistical Modeling: The Two Cultures



The Data Modeling Culture


The Algorithmic Modeling Culture


## Data and Models

From $\left\{\left(y_{i}, \boldsymbol{x}_{i}\right)\right\}$, there are different stories behind, see Freedman (2005)

- the causal story : $x_{j, i}$ is usually considered as independent of the other covariates $x_{k, i}$. For all possible $\boldsymbol{x}$, that value is mapped to $m(\boldsymbol{x})$ and a noise is attached, $\varepsilon$. The goal is to recover $m(\cdot)$, and the residuals are just the difference between the response value and $m(\boldsymbol{x})$.
- the conditional distribution story : for a linear model, we usually say that $Y$ given $\boldsymbol{X}=\boldsymbol{x}$ is a $\mathcal{N}\left(m(\boldsymbol{x}), \sigma^{2}\right)$ distribution. $m(\boldsymbol{x})$ is then the conditional mean. Here $m(\cdot)$ is assumed to really exist, but no causal assumption is made, only a conditional one.
- the explanatory data story : there is no model, just data. We simply want to summarize information contained in $\boldsymbol{x}$ 's to get an accurate summary, close to the response (i.e. $\min \{\ell(\boldsymbol{y}, m(\boldsymbol{x}))\})$ for some loss function $\ell$.

See also Varian (2014)

## Data, Models \& Causal Inference

We cannot differentiate data and model that easily.
After an operation, should I stay at hospital, or go back home ? as in Angrist \& Pischke (2008),
(health | hospital) - (health | stayed home)
should be written

$$
\begin{array}{lr}
\text { (health } \mid \text { hospital })-(\text { health } \mid \text { had stayed home }) & \text { [treatment effect] } \\
+(\text { health } \mid \text { had stayed home })-(\text { health } \mid \text { stayed home }) & \text { [selection bias] }
\end{array}
$$

Need randomization to solve selection bias.

## Econometric Modeling

Data $\left\{\left(y_{i}, \boldsymbol{x}_{i}\right)\right\}$, for $i=1, \cdots, n$, with $\boldsymbol{x}_{i} \in \mathcal{X} \subset \mathbb{R}^{p}$ and $y_{i} \in \mathcal{Y}$.
A model is a $m: \mathcal{X} \mapsto \mathcal{Y}$ mapping

- regression, $\mathcal{Y}=\mathbb{R}$ (but also $\mathcal{Y}=\mathbb{N}$ )
- classification, $\mathcal{Y}=\{0,1\},\{-1,+1\},\{\bullet \bullet \bullet\}$ (binary, or more)

Classification models are based on two steps,

- score function, $s(\boldsymbol{x})=\mathbb{P}(Y=1 \mid \boldsymbol{X}=\boldsymbol{x}) \in[0,1]$

- classifier $s(\boldsymbol{x}) \rightarrow \widehat{y} \in\{0,1\}$.


## High Dimensional Data (not to say 'Big Data')

See Bühlmann \& van de Geer (2011) or Koch (2013), $\boldsymbol{X}$ is a $n \times p$ matrix Portnoy (1988) proved that maximum likelihood estimators are asymptotically normal when $p^{2} / n \rightarrow 0$ as $n, p \rightarrow \infty$. Hence, massive data, when $p>\sqrt{n}$.

More intersting is the sparcity concept, based not on $p$, but on the effective size. Hence one can have $p>n$ and convergent estimators.

High dimension might be scary because of curse of dimensionality, see Bellman (1957). The volume of the unit sphere in $\mathbb{R}^{p}$ tends to 0 as $p \rightarrow \infty$, i.e.space is sparse.

## Computational \& Nonparametric Econometrics

Linear Econometrics: estimate $g: \boldsymbol{x} \mapsto \mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]$ by a linear function.
Nonlinear Econometrics: consider the approximation for some functional basis

$$
g(\boldsymbol{x})=\sum_{j=0}^{\infty} \omega_{j} g_{j}(\boldsymbol{x}) \text { and } \widehat{g}(\boldsymbol{x})=\sum_{j=0}^{h} \omega_{j} g_{j}(\boldsymbol{x})
$$

or consider a local model, on the neighborhood of
$\boldsymbol{x}$,
$\widehat{g}(x)=\frac{1}{n_{\boldsymbol{x}}} \sum_{i \in \mathcal{I}_{\boldsymbol{x}}} y_{i}$, with $\mathcal{I}_{\boldsymbol{x}}=\left\{\boldsymbol{x} \in \mathbb{R}^{p}:\left\|\boldsymbol{x}_{i}-\boldsymbol{x}\right\| \leq h\right\}$,
see Nadaraya (1964) and Watson (1964).
Here $h$ is some tunning parameter: not estimated, but chosen (optimaly).

## Econometrics \& Probabilistic Model

The primary goal in a regression analysis is to understand, as far as possible with the available data, how the conditional distribution of the response $y$ varies across subpopulations determined by the possible values of the predictor or predictors. Since this is the central idea, it will be helpful to have a conve-
from Cook \& Weisberg (1999), see also Haavelmo (1965).

$$
(Y \mid \boldsymbol{X}=\boldsymbol{x}) \sim \mathcal{N}\left(\mu(\boldsymbol{x}), \sigma^{2}\right) \text { with } \mu(\boldsymbol{x})=\beta_{0}+\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}, \text { and } \boldsymbol{\beta} \in \mathbb{R}^{p}
$$

Linear Model: $\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=\beta_{0}+\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}$
Homoscedasticity: $\operatorname{Var}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=\sigma^{2}$.

## Conditional Distribution and Likelihood

$$
(Y \mid \boldsymbol{X}=\boldsymbol{x}) \sim \mathcal{N}\left(\mu(\boldsymbol{x}), \sigma^{2}\right) \text { with } \mu(\boldsymbol{x})=\beta_{0}+\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}, \text { et } \boldsymbol{\beta} \in \mathbb{R}^{p}
$$

The log-likelihood is

$$
\log \mathcal{L}\left(\beta_{0}, \boldsymbol{\beta}, \sigma^{2} \mid \boldsymbol{y}, \boldsymbol{x}\right)=-\frac{n}{2} \log \left[2 \pi \sigma^{2}\right]-\frac{1}{2 \sigma^{2}} \underbrace{\sum_{i=1}^{n}\left(y_{i}-\beta_{0}-\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}\right)^{2}} .
$$

Set

$$
\left(\widehat{\beta}_{0}, \widehat{\boldsymbol{\beta}}, \widehat{\sigma}^{2}\right)=\operatorname{argmax}\left\{\log \mathcal{L}\left(\beta_{0}, \boldsymbol{\beta}, \sigma^{2} \mid \boldsymbol{y}, \boldsymbol{x}\right)\right\} .
$$

First order condition $\boldsymbol{X}^{\top}[\boldsymbol{y}-\boldsymbol{X} \widehat{\boldsymbol{\beta}}]=0$. If matrix $\boldsymbol{X}$ is a full rank matrix

$$
\widehat{\boldsymbol{\beta}}=\left(\boldsymbol{X}^{\top} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^{\top} \boldsymbol{y}=\boldsymbol{\beta}+\left(\boldsymbol{X}^{\top} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^{\top} \boldsymbol{\varepsilon}
$$

Asymptotic properties of $\widehat{\boldsymbol{\beta}}$,

$$
\sqrt{n}(\widehat{\boldsymbol{\beta}}-\boldsymbol{\beta}) \xrightarrow{\mathcal{L}} \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}) \text { as } n \rightarrow \infty
$$

## Geometric Perspective

Define the orthogonal projection on $\mathcal{X}$,

$$
\begin{gathered}
\Pi_{\boldsymbol{X}}=\boldsymbol{X}\left[\boldsymbol{X}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top} \\
\widehat{\boldsymbol{y}}=\underbrace{\boldsymbol{X}\left[\boldsymbol{X}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top}}_{\Pi_{\boldsymbol{X}}} \boldsymbol{y}=\Pi_{\boldsymbol{X}} \boldsymbol{y} .
\end{gathered}
$$



Pythagoras' theorem can be writen

$$
\|\boldsymbol{y}\|^{2}=\left\|\Pi_{\boldsymbol{X}} \boldsymbol{y}\right\|^{2}+\left\|\Pi_{\boldsymbol{X}^{\perp}} \boldsymbol{y}\right\|^{2}=\left\|\Pi_{\boldsymbol{X}} \boldsymbol{y}\right\|^{2}+\left\|\boldsymbol{y}-\Pi_{\boldsymbol{X}} \boldsymbol{y}\right\|^{2}
$$

which can be expressed as

$$
\underbrace{\sum_{i=1}^{n} y_{i}^{2}}_{n \times \text { total variance }}=\underbrace{\sum_{i=1}^{n} \widehat{y}_{i}^{2}}_{n \times \operatorname{explained} \text { variance }}+\underbrace{\sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}}_{n \times \text { residual variance }}
$$

## Geometric Perspective

Define the angle $\theta$ between $\boldsymbol{y}$ and $\Pi_{\mathcal{X}} \boldsymbol{y}$,

$$
R^{2}=\frac{\left\|\Pi_{\mathcal{X}} \boldsymbol{y}\right\|^{2}}{\|\boldsymbol{y}\|^{2}}=1-\frac{\left\|\Pi_{\mathcal{X} \perp} \boldsymbol{y}\right\|^{2}}{\|\boldsymbol{y}\|^{2}}=\cos ^{2}(\theta)
$$

see Davidson \& MacKinnon (2003)

$$
\boldsymbol{y}=\beta_{0}+\boldsymbol{X}_{1} \boldsymbol{\beta}_{1}+\boldsymbol{X}_{2} \boldsymbol{\beta}_{2}+\varepsilon
$$

If $\boldsymbol{y}_{2}^{\star}=\Pi_{\mathcal{X}_{1}^{\perp}} \boldsymbol{y}$ and $\boldsymbol{X}_{2}^{\star}=\Pi_{\mathcal{X}_{1}^{\perp}} \boldsymbol{X}_{2}$, then

$$
\widehat{\boldsymbol{\beta}}_{2}=\left[\boldsymbol{X}_{2}^{\star \top} \boldsymbol{X}_{2}^{\star}\right]^{-1} \boldsymbol{X}_{2}^{\star \top} \boldsymbol{y}_{2}^{\star}
$$

$\boldsymbol{X}_{2}^{\star}=\boldsymbol{X}_{2}$ if $\boldsymbol{X}_{1} \perp \boldsymbol{X}_{2}$,
Frisch-Waugh theorem.


## From Linear to Non-Linear

$$
\widehat{\boldsymbol{y}}=\boldsymbol{X} \widehat{\boldsymbol{\beta}}=\underbrace{\boldsymbol{X}\left[\boldsymbol{X}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top}}_{\boldsymbol{H}} \boldsymbol{y} \text { i.e. } \widehat{y}_{i}=\boldsymbol{h}_{\boldsymbol{x}_{i}}^{\top} \boldsymbol{y}
$$

with - for the linear regression - $\boldsymbol{h}_{\boldsymbol{x}}=\boldsymbol{X}\left[\boldsymbol{X}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{x}$.
One can consider some smoothed regression, see Nadaraya (1964) and Watson (1964), with some smoothing matrix $\boldsymbol{S}$

$$
\widehat{m}_{h}(x)=\boldsymbol{s}_{x}^{\top} \boldsymbol{y}=\sum_{i=1}^{n} s_{x, i} y_{i} \text { withs } s_{x, i}=\frac{K_{h}\left(x-x_{i}\right)}{K_{h}\left(x-x_{1}\right)+\cdots+K_{h}\left(x-x_{n}\right)}
$$

for some kernel $K(\cdot)$ and some bandwidth $h>0$.

## From Linear to Non-Linear

$$
T=\frac{\|\boldsymbol{S} \boldsymbol{y}-\boldsymbol{H} \boldsymbol{y}\|}{\operatorname{trace}\left([\boldsymbol{S}-\boldsymbol{H}]^{\top}[\boldsymbol{S}-\boldsymbol{H}]\right)}
$$

can be used to test for linearity, Simonoff (1996). trace $(\boldsymbol{S})$ is the equivalent number of parameters, and $n-\operatorname{trace}(\boldsymbol{S})$ the degrees of freedom, Ruppert et al. (2003).

Nonlinear Model, but Homoscedastic - Gaussian

- $(Y \mid \boldsymbol{X}=\boldsymbol{x}) \sim \mathcal{N}\left(\mu(\boldsymbol{x}), \sigma^{2}\right)$
- $\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=\mu(\boldsymbol{x})$


## Conditional Expectation


from Angrist \& Pischke (2008), $\boldsymbol{x} \mapsto \mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]$.

## Exponential Distributions and Linear Models

$$
f\left(y_{i} \mid \theta_{i}, \phi\right)=\exp \left(\frac{y_{i} \theta_{i}-b\left(\theta_{i}\right)}{a(\phi)}+c\left(y_{i}, \phi\right)\right) \text { with } \theta_{i}=h\left(\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}\right)
$$

Log likelihood is expressed as

$$
\log \mathcal{L}(\boldsymbol{\theta}, \phi \mid \boldsymbol{y})=\sum_{i=1}^{n} \log f\left(y_{i} \mid \theta_{i}, \phi\right)=\frac{\sum_{i=1}^{n} y_{i} \theta_{i}-\sum_{i=1}^{n} b\left(\theta_{i}\right)}{a(\phi)}+\sum_{i=1}^{n} c\left(y_{i}, \phi\right)
$$

and first order conditions

$$
\frac{\partial \log \mathcal{L}(\boldsymbol{\theta}, \phi \mid \boldsymbol{y})}{\partial \boldsymbol{\beta}}=\boldsymbol{X}^{\top} \boldsymbol{W}^{-1}[\boldsymbol{y}-\boldsymbol{\mu}]=\mathbf{0}
$$

as in Müller (2001), where $\boldsymbol{W}$ is a weight matrix, function of $\boldsymbol{\beta}$.
We usually specify the link function $g(\cdot)$ defined as

$$
\widehat{y}=m(\boldsymbol{x})=\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=g^{-1}\left(\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}\right)
$$

## Exponential Distributions and Linear Models

Note that $\boldsymbol{W}=\operatorname{diag}(\nabla g(\widehat{\boldsymbol{y}}) \cdot \operatorname{Var}[\boldsymbol{y}])$, and set

$$
\boldsymbol{z}=g(\widehat{\boldsymbol{y}})+(\boldsymbol{y}-\widehat{\boldsymbol{y}}) \cdot \nabla g(\widehat{\boldsymbol{y}})
$$

the the maximum likelihood estimator is obtained iteratively

$$
\widehat{\boldsymbol{\beta}}_{k+1}=\left[\boldsymbol{X}^{\top} \boldsymbol{W}_{k}^{-1} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top} \boldsymbol{W}_{k}^{-1} \boldsymbol{z}_{k}
$$

Set $\widehat{\boldsymbol{\beta}}=\boldsymbol{\beta}_{\infty}$, so that

$$
\sqrt{n}(\widehat{\boldsymbol{\beta}}-\boldsymbol{\beta}) \stackrel{\mathcal{L}}{\rightarrow} \mathcal{N}\left(\mathbf{0}, I(\boldsymbol{\beta})^{-1}\right)
$$

with $I(\boldsymbol{\beta})=\phi \cdot\left[\boldsymbol{X}^{\top} \boldsymbol{W}_{\infty}^{-1} \boldsymbol{X}\right]$.
Note that $\left[\boldsymbol{X}^{\top} \boldsymbol{W}_{k}^{-1} \boldsymbol{X}\right]$ is a $p \times p$ matrix.

## Exponential Distributions and Linear Models

Generalized Linear Model:

- $(Y \mid \boldsymbol{X}=\boldsymbol{x}) \sim \mathcal{L}\left(\theta_{\boldsymbol{x}}, \varphi\right)$
- $\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=h^{-1}\left(\theta_{\boldsymbol{x}}\right)=g^{-1}\left(\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}\right)$
e.g. $(Y \mid \boldsymbol{X}=\boldsymbol{x}) \sim \mathcal{P}\left(\exp \left[\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}\right]\right)$.

Use of maximum likelihood techniques for inference.

Actually, more a moment condition than a distribution assumption.

## Goodness of Fit \& Model Choice

From the variance decomposition

$$
\underbrace{\frac{1}{n} \sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}_{\text {total variance }}=\underbrace{\frac{1}{n} \sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}}_{\text {residual variance }}+\underbrace{\frac{1}{n} \sum_{i=1}^{n}\left(\widehat{y}_{i}-\bar{y}\right)^{2}}_{\text {explained variance }}
$$

and define

$$
R^{2}=\frac{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}-\sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}}{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}
$$

More generally

$$
\text { Deviance }(\boldsymbol{\beta})=-2 \log [\mathcal{L}]=2 \sum_{i=1}\left(y_{i}-\widehat{y}_{i}\right)^{2}=\operatorname{Deviance}(\widehat{\boldsymbol{y}})
$$

The null deviance is obtained using $\widehat{y}_{i}=\bar{y}$, so that

$$
R^{2}=\frac{\operatorname{Deviance}(\bar{y})-\operatorname{Deviance}(\widehat{\boldsymbol{y}})}{\operatorname{Deviance}(\bar{y})}=1-\frac{\operatorname{Deviance}(\widehat{\boldsymbol{y}})}{\operatorname{Deviance}(\bar{y})}=1-\frac{\mathrm{D}}{\mathrm{D}_{0}}
$$

## Goodness of Fit \& Model Choice

One usually prefers a penalized version

$$
\bar{R}^{2}=1-\left(1-R^{2}\right) \frac{n-1}{n-p}=R^{2}-\underbrace{\left(1-R^{2}\right) \frac{p-1}{n-p}}_{\text {penalty }}
$$

See also Akaike criteria $A I C=$ Deviance $+2 \cdot p$
or Schwarz, $B I C=$ Deviance $+\log (n) \cdot p$
In high dimension, consider a corrected version

$$
A I C c=\text { Deviance }+2 \cdot p \cdot \frac{n}{n-p-1}
$$

## Stepwise Procedures

Forward algorithm

1. set $j_{1}^{\star}=\underset{j \in\{\emptyset, 1, \cdots, n\}}{\operatorname{argmin}}\{\operatorname{AIC}(\{j\})\}$
2. set $j_{2}^{\star}=\underset{j \in\{\emptyset, 1, \cdots, n\} \backslash\left\{j_{1}^{\star}\right\}}{\operatorname{argmin}}\left\{\operatorname{AIC}\left(\left\{j_{1}^{\star}, j\right\}\right)\right\}$
3. ... until $j^{\star}=\emptyset$

Backward algorithm

1. set $j_{1}^{\star}=\underset{j \in\{\emptyset, 1, \cdots, n\}}{\operatorname{argmin}}\{\operatorname{AIC}(\{1, \cdots, n\} \backslash\{j\})\}$
2. set $j_{2}^{\star}=\underset{j \in\{\emptyset, 1, \cdots, n\} \backslash\left\{j_{1}^{\star}\right\}}{\operatorname{argmin}}\left\{\operatorname{AIC}\left(\{1, \cdots, n\} \backslash\left\{j_{1}^{\star}, j\right\}\right)\right\}$
3. ... until $j^{\star}=\emptyset$

## Econometrics \& Statistical Testing

Standard test for $H_{0}: \beta_{k}=0$ against $H_{1}: \beta_{k} \neq 0$ is Student- $t$ est $t_{k}=\widehat{\beta}_{k} / \mathrm{se}_{\widehat{\beta}_{k}}$,
Use the $p$-value $\mathbb{P}\left[|T|>\left|t_{k}\right|\right]$ with $T \sim t_{\nu}($ and $\nu=\operatorname{trace}(\boldsymbol{H})$ ).
In high dimension, consider the FDR (False Discovery Ratio).
With $\alpha=5 \%, 5 \%$ variables are wrongly significant.
If $p=100$ with only 5 significant variables, one should expect also 5 false positive, i.e. $50 \%$ FDR, see Benjamini \& Hochberg (1995) and Andrew Gelman's talk.

## Under \& Over-Identification

Under-identification is obtained when the true model is $y=\beta_{0}+\boldsymbol{x}_{1}^{\top} \boldsymbol{\beta}_{1}+\boldsymbol{x}_{2}^{\top} \boldsymbol{\beta}_{2}+\varepsilon$, but we estimate $y=\beta_{0}+\boldsymbol{x}_{1}^{\top} \boldsymbol{b}_{1}+\eta$.

Maximum likelihood estimator for $\boldsymbol{b}_{1}$ is

$$
\begin{aligned}
\widehat{\boldsymbol{b}}_{1} & =\left(\boldsymbol{X}_{1}^{\top} \boldsymbol{X}_{1}\right)^{-1} \boldsymbol{X}_{1}^{\top} \boldsymbol{y} \\
& =\left(\boldsymbol{X}_{1}^{\top} \boldsymbol{X}_{1}\right)^{-1} \boldsymbol{X}_{1}^{\top}\left[\boldsymbol{X}_{1, i} \boldsymbol{\beta}_{1}+\boldsymbol{X}_{2, i} \boldsymbol{\beta}_{2}+\varepsilon\right] \\
& =\boldsymbol{\beta}_{1}+\underbrace{\left(\boldsymbol{X}_{1}^{\prime} \boldsymbol{X}_{1}\right)^{-1} \boldsymbol{X}_{1}^{\top} \boldsymbol{X}_{2} \boldsymbol{\beta}_{2}}_{\boldsymbol{\beta}_{12}}+\underbrace{\left(\boldsymbol{X}_{1}^{\top} \boldsymbol{X}_{1}\right)^{-1} \boldsymbol{X}_{1}^{\top} \varepsilon}_{\nu_{i}}
\end{aligned}
$$

so that $\mathbb{E}\left[\widehat{\boldsymbol{b}}_{1}\right]=\boldsymbol{\beta}_{1}+\boldsymbol{\beta}_{12}$, and the bias is null when $\boldsymbol{X}_{1}^{\top} \boldsymbol{X}_{2}=\mathbf{0}$ i.e. $\boldsymbol{X}_{1} \perp \boldsymbol{X}_{2}$, see Frisch-Waugh).
Over-identification is obtained when the true model is $y=\beta_{0}+\boldsymbol{x}_{1}^{\top} \boldsymbol{\beta}_{1} \varepsilon$, but we fit $y=\beta_{0}+\boldsymbol{x}_{1}^{\boldsymbol{\top}} \boldsymbol{b}_{1}+\boldsymbol{x}_{2}^{\boldsymbol{\top}} \boldsymbol{b}_{2}+\eta$.

Inference is unbiased since $\mathbb{E}\left(\boldsymbol{b}_{1}\right)=\boldsymbol{\beta}_{1}$ but the estimator is not efficient.

## Statistical Learning \& Loss Function

Here, no probabilistic model, but a loss function, $\ell$. For some set of functions $\mathcal{M}, \mathcal{X} \rightarrow \mathcal{Y}$, define

$$
m^{\star}=\underset{m \in \mathcal{M}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell\left(y_{i}, m\left(\boldsymbol{x}_{i}\right)\right)\right\}
$$

Quadratic loss functions are interesting since

$$
\bar{y}=\underset{m \in \mathbb{R}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \frac{1}{n}\left[y_{i}-m\right]^{2}\right\}
$$

which can be writen, with some underlying probabilistic model

$$
\mathbb{E}(Y)=\underset{m \in \mathbb{R}}{\operatorname{argmin}}\left\{\|Y-m\|_{\ell_{2}}^{2}\right\}=\underset{m \in \mathbb{R}}{\operatorname{argmin}}\left\{\mathbb{E}\left([Y-m]^{2}\right)\right\}
$$

For $\tau \in(0,1)$, we obtain the quantile regression (see Koenker (2005))

$$
m^{\star}=\underset{m \in \mathcal{M}_{0}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell_{\tau}\left(y_{i}, m\left(\boldsymbol{x}_{i}\right)\right)\right\} \operatorname{avec} \ell_{\tau}(x, y)=\left|(x-y)\left(\tau-\mathbf{1}_{x \leq y}\right)\right|
$$

## Boosting \& Weak Learning

$$
m^{\star}=\underset{m \in \mathcal{M}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell\left(y_{i}, m\left(\boldsymbol{x}_{i}\right)\right)\right\}
$$

is hard to solve for some very large and general space $\mathcal{M}$ of $\mathcal{X} \rightarrow \mathcal{Y}$ functions.
Consider some iterative procedure, where we learn from the errors,

$$
m^{(k)}(\cdot)=\underbrace{m_{1}(\cdot)}_{\sim \boldsymbol{y}}+\underbrace{m_{2}(\cdot)}_{\sim \varepsilon_{1}}+\underbrace{m_{3}(\cdot)}_{\sim \varepsilon_{2}}+\cdots+\underbrace{m_{k}(\cdot)}_{\sim \varepsilon_{k-1}}=m^{(k-1)}(\cdot)+m_{k}(\cdot)
$$

Formely $\varepsilon$ can be seen as $\nabla \ell$, the gradient of the loss.

## Boosting \& Weak Learning

It is possible to see this algorithm as a gradient descent. Not

$$
\underbrace{f\left(\boldsymbol{x}_{k}\right)}_{\left\langle f, \boldsymbol{x}_{k}\right\rangle} \sim \underbrace{f\left(\boldsymbol{x}_{k-1}\right)}_{\left\langle f, \boldsymbol{x}_{k-1}\right\rangle}+\underbrace{\left(\boldsymbol{x}_{k}-\boldsymbol{x}_{k-1}\right)}_{\alpha_{k}} \underbrace{\nabla f\left(\boldsymbol{x}_{k-1}\right)}_{\left\langle\nabla f, \boldsymbol{x}_{k-1}\right\rangle}
$$

but some kind of dual version

$$
\underbrace{f_{k}(\boldsymbol{x})}_{\left\langle f_{k}, \boldsymbol{x}\right\rangle} \sim \underbrace{f_{k-1}(\boldsymbol{x})}_{\left\langle f_{k-1}, \boldsymbol{x}\right\rangle}+\underbrace{\left(f_{k}-f_{k-1}\right)}_{a_{k}} \underbrace{\star}_{\left\langle f_{k-1}, \nabla \boldsymbol{x}\right\rangle}
$$

where $\star$ is a gradient is some functional space.

$$
m^{(k)}(\boldsymbol{x})=m^{(k-1)}(\boldsymbol{x})+\underset{f \in \mathcal{F}}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell\left(y_{i}, m^{(k-1)}(\boldsymbol{x})+f(\boldsymbol{x})\right)\right\}
$$

for some simple space $\mathcal{F}$ so that we define some weak learner, e.g. step functions (so called stumps)

## Boosting \& Weak Learning

Standard set $\mathcal{F}$ are stumps functions but one can also consider splines (with non-fixed knots).

One might add a shrinkage parameter to learn even more weakly, i.e. set $\varepsilon_{1}=y-\alpha \cdot m_{1}(\boldsymbol{x})$ with $\alpha \in(0,1)$, etc.

## Big Data \& Linear Model

Consider some linear model $y_{i}=\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}+\varepsilon_{i}$ for all $i=1, \cdots, n$.
Assume that $\varepsilon_{i}$ are i.i.d. with $\mathbb{E}(\varepsilon)=0$ (and finite variance). Write

$$
\underbrace{\left(\begin{array}{c}
y_{1} \\
\vdots \\
y_{n}
\end{array}\right)}_{\boldsymbol{y}, n \times 1}=\underbrace{\left(\begin{array}{cccc}
1 & x_{1,1} & \cdots & x_{1, p} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_{n, 1} & \cdots & x_{n, p}
\end{array}\right)}_{\boldsymbol{X}, n \times(p+1)} \underbrace{\left(\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\vdots \\
\beta_{p}
\end{array}\right)}_{\boldsymbol{\beta},(p+1) \times 1}+\underbrace{\left(\begin{array}{c}
\varepsilon_{1} \\
\vdots \\
\varepsilon_{n}
\end{array}\right)}_{\varepsilon, n \times 1} .
$$

Assuming $\varepsilon \sim \mathcal{N}\left(\mathbf{0}, \sigma^{2} \mathbb{I}\right)$, the maximum likelihood estimator of $\boldsymbol{\beta}$ is

$$
\widehat{\boldsymbol{\beta}}=\operatorname{argmin}\left\{\left\|\boldsymbol{y}-\boldsymbol{X}^{\boldsymbol{\top}} \boldsymbol{\beta}\right\|_{\ell_{2}}\right\}=\left(\boldsymbol{X}^{\top} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^{\boldsymbol{\top}} \boldsymbol{y}
$$

... under the assumtption that $\boldsymbol{X}^{\top} \boldsymbol{X}$ is a full-rank matrix.
What if $\boldsymbol{X}^{\top} \boldsymbol{X}$ cannot be inverted? Then $\widehat{\boldsymbol{\beta}}=\left[\boldsymbol{X}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top} \boldsymbol{y}$ does not exist, but $\widehat{\boldsymbol{\beta}}_{\lambda}=\left[\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \mathbb{I}\right]^{-1} \boldsymbol{X}^{\top} \boldsymbol{y}$ always exist if $\lambda>0$.

## Ridge Regression \& Regularization

The estimator $\widehat{\boldsymbol{\beta}}=\left[\boldsymbol{X}^{\top} \boldsymbol{X}+\lambda \mathbb{I}\right]^{-1} \boldsymbol{X}^{\top} \boldsymbol{y}$ is the Ridge estimate obtained as solution of

$$
\widehat{\boldsymbol{\beta}}=\underset{\boldsymbol{\beta}}{\operatorname{argmin}}\{\sum_{i=1}^{n}\left[y_{i}-\beta_{0}-\boldsymbol{x}_{i}^{\boldsymbol{\top}} \boldsymbol{\beta}\right]^{2}+\lambda \underbrace{\|\boldsymbol{\beta}\|_{\ell_{2}}^{2}}_{\mathbf{1}^{\top} \boldsymbol{\beta}^{2}}\}
$$

for some tuning parameter $\lambda$. One can also write

$$
\widehat{\boldsymbol{\beta}}=\underset{\boldsymbol{\beta} ;\|\boldsymbol{\beta}\|_{\ell_{2}} \leq s}{\operatorname{argmin}}\left\{\left\|\boldsymbol{Y}-\boldsymbol{X}^{\boldsymbol{\top}} \boldsymbol{\beta}\right\|_{\ell_{2}}\right\}
$$

There is a Bayesian interpretation of that regularization, when $\boldsymbol{\beta}$ has some prior $\mathcal{N}\left(\boldsymbol{\beta}_{0}, \tau \mathbb{I}\right)$.

## Over-Fitting \& Penalization

Solve here, for some norm $\|\cdot\|$,

$$
\min \left\{\sum_{i=1}^{n} \ell\left(y_{i}, \beta_{0}+\boldsymbol{x}^{\top} \boldsymbol{\beta}\right)+\lambda\|\boldsymbol{\beta}\|\right\}=\min \{\operatorname{objective}(\boldsymbol{\beta})+\text { penality }(\boldsymbol{\beta})\} .
$$

Estimators are no longer unbiased, but might have a smaller mse.
Consider some i.id. sample $\left\{y_{1}, \cdots, y_{n}\right\}$ from $\mathcal{N}\left(\theta, \sigma^{2}\right)$, and consider some estimator proportional to $\bar{y}$, i.e. $\widehat{\theta}=\alpha \bar{y}$. $\alpha=1$ is the maximum likelihood estimator.

Note that

$$
\operatorname{mse}[\hat{\theta}]=\underbrace{(\alpha-1)^{2} \mu^{2}}_{\operatorname{bias}[\hat{\theta}]^{2}}+\underbrace{\frac{\alpha^{2} \sigma^{2}}{n}}_{\operatorname{Var}[\hat{\theta}]}
$$

and $\alpha^{\star}=\mu^{2} \cdot\left(\mu^{2}+\frac{\sigma^{2}}{n}\right)^{-1}<1$.

$$
\left(\widehat{\beta}_{0}, \widehat{\boldsymbol{\beta}}\right)=\operatorname{argmin}\left\{\sum_{i=1}^{n} \ell\left(y_{i}, \beta_{0}+\boldsymbol{x}^{\top} \boldsymbol{\beta}\right)+\lambda\|\beta\|\right\}
$$

can be seen as a Lagrangian minimization problem

$$
\left(\widehat{\beta}_{0}, \widehat{\boldsymbol{\beta}}\right)=\underset{\boldsymbol{\beta} ;\|\boldsymbol{\beta}\| \leq s}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \ell\left(y_{i}, \beta_{0}+\boldsymbol{x}^{\top} \boldsymbol{\beta}\right)\right\}
$$





## LASSO \& Sparcity

In severall applications, $p$ can be (very) large, but a lot of features are just noise: $\beta_{j}=0$ for many $j$ 's. Let $s$ denote the number of relevent features, with $s \ll p$, cf Hastie, Tibshirani \& Wainwright (2015),

$$
s=\operatorname{card}\{\mathcal{S}\} \text { where } \mathcal{S}=\left\{j ; \beta_{j} \neq 0\right\}
$$

The true model is now $y=\boldsymbol{X}_{\mathcal{S}}^{\top} \boldsymbol{\beta}_{\mathcal{S}}+\varepsilon$, where $\boldsymbol{X}_{\mathcal{S}}^{\top} \boldsymbol{X}_{\mathcal{S}}$ is a full rank matrix.

## LASSO \& Sparcity

Evoluation of $\widehat{\boldsymbol{\beta}}_{\lambda}$ as a function of $\log \lambda$ in various applications



## In-Sample \& Out-Sample

Write $\widehat{\boldsymbol{\beta}}=\widehat{\boldsymbol{\beta}}\left(\left(\boldsymbol{x}_{1}, y_{1}\right), \cdots,\left(\boldsymbol{x}_{n}, y_{n}\right)\right)$. Then (for the linear model)

$$
\text { Deviance is }(\widehat{\boldsymbol{\beta}})=\sum_{i=1}^{n}\left[y_{i}-\boldsymbol{x}_{i}^{\top} \widehat{\boldsymbol{\beta}}\left(\left(\boldsymbol{x}_{1}, y_{1}\right), \cdots,\left(\boldsymbol{x}_{n}, y_{n}\right)\right)\right]^{2}
$$

Withe this "in-sample" deviance, we cannot use the central limit theorem

$$
\frac{\text { Deviance }_{\text {Is }}(\widehat{\boldsymbol{\beta}})}{n} \nrightarrow \mathbb{E}\left(\left[Y-\boldsymbol{X}^{\boldsymbol{\top}} \boldsymbol{\beta}\right]\right)
$$

Hence, we can compute some "out-of-sample" deviance

$$
\text { Deviance os }(\widehat{\boldsymbol{\beta}})=\sum_{i=n+1}^{m+n}\left[y_{i}-\boldsymbol{x}_{i}^{\boldsymbol{\top}} \widehat{\boldsymbol{\beta}}\left(\left(\boldsymbol{x}_{1}, y_{1}\right), \cdots,\left(\boldsymbol{x}_{n}, y_{n}\right)\right]^{2}\right.
$$

## In-Sample \& Out-Sample

Observe that there are connexions with Akaike penaly function

$$
\text { Deviance is }(\widehat{\boldsymbol{\beta}})-\text { Deviance os }(\widehat{\boldsymbol{\beta}}) \approx 2 \cdot \text { degrees of freedom }
$$

From Stone (1977), minimizing AIC is closed to cross validation,

From Shao (1997) minimizing BIC is closed to $k$-fold cross validation with $k=n / \log n$.


## Overfit, Generalization \& Model Complexity

Complexity of the model is the degree of the polynomial function

## Cross-Validation

See Jacknife technique Quenouille (1956) or Tukey (1958) to reduce the bias.
If $\left\{y_{1}, \cdots, y_{n}\right\}$ is an i.id. sample from $F_{\theta}$, with estimator $T_{n}(\boldsymbol{y})=T_{n}\left(y_{1}, \cdots, y_{n}\right)$, such that $\mathbb{E}\left[T_{n}(\boldsymbol{Y})\right]=\theta+O\left(n^{-1}\right)$, consider

$$
\widetilde{T}_{n}(\boldsymbol{y})=\frac{1}{n} \sum_{i=1}^{n} T_{n-1}\left(\boldsymbol{y}_{(i)}\right) \text { avec } \boldsymbol{y}_{(i)}=\left(y_{1}, \cdots, y_{i-1}, y_{i+1}, \cdots, y_{n}\right)
$$

Then $\mathbb{E}\left[\widetilde{T}_{n}(\boldsymbol{Y})\right]=\theta+O\left(n^{-2}\right)$.
Similar idea in leave-one-out cross validation

$$
\text { Risk }=\frac{1}{n} \sum_{i=1}^{n} \ell\left(y_{i}, \widehat{m}_{(i)}\left(\boldsymbol{x}_{i}\right)\right)
$$

## Rule of Thumb vs. Cross Validation

$\widehat{m}^{\left[h^{\star}\right]}(x)=\widehat{\beta}_{0}^{[x]}+\widehat{\beta}_{1}^{[x]} x$ with $\left(\widehat{\beta}_{0}^{[x]}, \widehat{\beta}_{1}^{[x]}\right)=\underset{\left(\beta_{0}, \beta_{1}\right)}{\operatorname{argmin}}\left\{\sum_{i=1}^{n} \omega_{h^{\star}}^{[x]}\left[y_{i}-\left(\beta_{0}+\beta_{1} x_{i}\right)\right]^{2}\right\}$

set $h^{\star}=\operatorname{argmin}\{\operatorname{mse}(h)\}$ with $\operatorname{mse}(h)=\frac{1}{n} \sum_{i=1}^{n}\left[y_{i}-\widehat{m}_{(i)}^{[h]}\left(x_{i}\right)\right]^{2}$

## Exponential Smoothing for Time Series

Consider some exponential smoothing filter, on a time series $\left(x_{t}\right), \widehat{y}_{t+1}=\alpha \widehat{y}_{t}+(1-\alpha) y_{t}$, then consider

$$
\alpha^{\star}=\operatorname{argmin}\left\{\sum_{t=2}^{T} \ell\left(\widehat{y}_{t}, y_{t}\right)\right\},
$$

see Hyndman et al. (2003).

## Cross-Validation

Consider a partition of $\{1, \cdots, n\}$ in $k$ groups with the same size, $\mathcal{I}_{1}, \cdots, \mathcal{I}_{k}$, and set $\mathcal{I}_{\bar{j}}=\{1, \cdots, n\} \backslash \mathcal{I}_{j}$. Fit $\widehat{m}_{(j)}$ on $\mathcal{I}_{\bar{j}}$, and

$$
\text { Risk }=\frac{1}{k} \sum_{j=1}^{k} \operatorname{Risk}_{j} \text { where } \operatorname{Risk}_{j}=\frac{k}{n} \sum_{i \in \mathcal{I}_{j}} \ell\left(y_{i}, \widehat{m}_{(j)}\left(\boldsymbol{x}_{i}\right)\right)
$$

## Randomization is too important to be left to chance!

Consider some bootstraped sample, $\mathcal{I}_{b}=\left\{i_{1, b}, \cdots, i_{n, b}\right\}$, with $i_{k, b} \in\{1, \cdots, n\}$
Set $n_{i}=\mathbf{1}_{i \notin \mathcal{I}_{1}}+\cdots+\mathbf{1}_{i \notin v_{B}}$, and fit $\widehat{m}_{b}$ on $\mathcal{I}_{b}$

$$
\text { Risk }=\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{i}} \sum_{b: i \notin I_{b}} \ell\left(y_{i}, \widehat{m}_{b}\left(\boldsymbol{x}_{i}\right)\right)
$$

Probability that $i$ th obs. is not selection $\left(1-n^{-1}\right)^{n} \rightarrow e^{-1} \sim 36.8 \%$, see training / validation samples ( $2 / 3-1 / 3$ ).

## Bootstrap

From Efron (1987), generate samples from $\left(\Omega, \mathcal{F}, \mathbb{P}_{n}\right)$

$$
\widehat{F}_{n}(y)=\frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\left(y_{i} \leq y\right) \text { and } \widehat{F}_{n}\left(y_{i}\right)=\frac{\operatorname{rank}\left(y_{i}\right)}{n}
$$

If $U \sim \mathcal{U}([0,1]), F^{-1}(U) \sim F$
If $U \sim \mathcal{U}([0,1]), \widehat{F}_{n}^{-1}(U)$ is uniform
on $\left\{\frac{1}{n}, \cdots, \frac{n-1}{n}, 1\right\}$.
Consider some boostraped sample,

- either $\left(y_{i_{k}}, \boldsymbol{x}_{i_{k}}\right), i_{k} \in\{1, \cdots, n\}$
- or $\left(\widehat{y}_{k}+\widehat{\varepsilon}_{i_{k}}, \boldsymbol{x}_{k}\right), i_{k} \in\{1, \cdots, n\}$


## Classification \& Logistic Regression

Generalized Linear Model when $Y$ has a Bernoulli distribution, $y_{i} \in\{0,1\}$,

$$
m(\boldsymbol{x})=\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]=\frac{e^{\beta_{0}+\boldsymbol{x}^{\top} \boldsymbol{\beta}}}{1+e^{\beta_{0}+\boldsymbol{x}^{\top} \boldsymbol{\beta}}}=H\left(\beta_{0}+\boldsymbol{x}^{\boldsymbol{\top}} \boldsymbol{\beta}\right)
$$

Estimate $\left(\beta_{0}, \boldsymbol{\beta}\right)$ using maximum likelihood techniques

$$
\begin{aligned}
& \mathcal{L}=\prod_{i=1}^{n}\left(\frac{e^{\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}}}{1+e^{\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}}}\right)^{y_{i}}\left(\frac{1}{1+e^{\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}}}\right)^{1-y_{i}} \\
& \text { Deviance } \propto \sum_{i=1}^{n}\left[\log \left(1+e^{\boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}}\right)-y_{i} \boldsymbol{x}_{i}^{\top} \boldsymbol{\beta}\right]
\end{aligned}
$$

Observe that

$$
\mathrm{D}_{0} \propto \sum_{i=1}^{n}\left[y_{i} \log (\bar{y})+\left(1-y_{i}\right) \log (1-\bar{y})\right]
$$

## Classification Trees

To split $\{N\}$ into two $\left\{N_{L}, N_{R}\right\}$, consider

$$
\mathcal{I}\left(N_{L}, N_{R}\right)=\sum_{x \in\{L, R\}} \frac{n_{x}}{n} \mathcal{I}\left(N_{x}\right)
$$


e.g. Gini index (used originally in CART, see Breiman et al. (1984))

$$
\operatorname{gini}\left(N_{L}, N_{R}\right)=-\sum_{x \in\{L, R\}} \frac{n_{x}}{n} \sum_{y \in\{0,1\}} \frac{n_{x, y}}{n_{x}}\left(1-\frac{n_{x, y}}{n_{x}}\right)
$$

and the cross-entropy (used in C4.5 and C5.0)

$$
\operatorname{entropy}\left(N_{L}, N_{R}\right)=-\sum_{x \in\{L, R\}} \frac{n_{x}}{n} \sum_{y \in\{0,1\}} \frac{n_{x, y}}{n_{x}} \log \left(\frac{n_{x, y}}{n_{x}}\right)
$$

## Classification Trees



PRDIA


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$N_{L}:\left\{x_{i, j} \leq s\right\} \quad N_{R}:\left\{x_{i, j}>s\right\}$ solve $\max _{j \in\{1, \cdots, k\}, s}\left\{\mathcal{I}\left(N_{L}, N_{R}\right)\right\}$
$\longleftarrow$ first split




second split $\longrightarrow$


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## Trees \& Forests

Boostrap can be used to define the concept of margin,

$$
\operatorname{margin}_{i}=\frac{1}{B} \sum_{b=1}^{B} \mathbf{1}\left(\widehat{y}_{i}^{(b)}=y_{i}\right)-\frac{1}{B} \sum_{b=1}^{B} \mathbf{1}\left(\widehat{y}_{i}^{(b)} \neq y_{i}\right)
$$

Subsampling of variable, at each knot (e.g. $\sqrt{k}$ out of $k$ )
Concept of variable importance: given some random forest with $M$ trees,

$$
\text { importance of variable } k \quad I\left(X_{k}\right)=\frac{1}{M} \sum_{m} \sum_{t} \frac{N_{t}}{N} \Delta \mathcal{I}(t)
$$

where the first sum is over all trees, and the second one is over all nodes where the split is done based on variable $X_{k}$.

## Trees \& Forests



See also discriminant analysis, SVM, neural networks, etc.

## Model Selection \& ROC Curves

Given a scoring function $m(\cdot)$, with $m(\boldsymbol{x})=\mathbb{E}[Y \mid \boldsymbol{X}=\boldsymbol{x}]$, and a threshold $s \in(0,1)$, set

$$
\widehat{Y}^{(s)}=\mathbf{1}[m(\boldsymbol{x})>s]=\left\{\begin{array}{l}
1 \text { if } m(\boldsymbol{x})>s \\
0 \text { if } m(\boldsymbol{x}) \leq s
\end{array}\right.
$$

Define the confusion matrix as $\boldsymbol{N}=\left[N_{u, v}\right]$

$$
N_{u, v}^{(s)}=\sum_{i=1}^{n} \mathbf{1}\left(\widehat{y}_{i}^{(s)}=u, y_{j}=v\right) \text { for }(u, v) \in\{0,1\}
$$

|  | $Y=0$ | $Y=1$ |  |
| :---: | :---: | :---: | :---: |
| $\widehat{Y}_{s}=0$ | $\mathrm{TN}_{s}$ | $\mathrm{FN}_{s}$ | $\mathrm{TN}_{s}+\mathrm{FN}_{s}$ |
| $\widehat{Y}_{s}=1$ | $\mathrm{FP}_{s}$ | $\mathrm{TP}_{s}$ | $\mathrm{FP}_{s}+\mathrm{TP}_{s}$ |
|  | $\mathrm{TN}_{s}+\mathrm{FP}_{s}$ | $\mathrm{FN}_{s}+\mathrm{TP}_{s}$ | $n$ |

## Model Selection \& ROC Curves

ROC curve is

$$
\mathrm{ROC}_{s}=\left(\frac{\mathrm{FP}_{s}}{\mathrm{FP}_{s}+\mathrm{TN}_{s}}, \frac{\mathrm{TP}_{s}}{\mathrm{TP}_{s}+\mathrm{FN}_{s}}\right) \text { with } s \in(0,1)
$$

## Model Selection \& ROC Curves

In machine learning, the most popular measure is $\kappa$, see Landis \& Koch (1977). Define $\boldsymbol{N}^{\perp}$ from $\boldsymbol{N}$ as in the chi-square independence test. Set

$$
\begin{aligned}
& \qquad \text { total accuracy }=\frac{\mathrm{TP}+\mathrm{TN}}{n} \\
& \text { random accuracy }=\frac{\mathrm{TP}^{\perp}+\mathrm{TN}^{\perp}}{n}=\frac{[\mathrm{TN}+\mathrm{FP}] \cdot[\mathrm{TP}+\mathrm{FN}]+[\mathrm{TP}+\mathrm{FP}] \cdot[\mathrm{TN}+\mathrm{FN}]}{n^{2}} \\
& \text { and } \\
& \qquad \kappa=\frac{\text { total accuracy }- \text { random accuracy }}{1-\text { random accuracy }}
\end{aligned}
$$

See Kaggle competitions.

## Reducing Dimension with PCA

Use principal components to reduce dimension (on centered and scaled variables): we want $d$ vectors $\boldsymbol{z}_{1}, \cdots, \boldsymbol{z}_{d}$ such that

First Compoment is $\boldsymbol{z}_{1}=\boldsymbol{X} \boldsymbol{\omega}_{1}$ where

$$
\boldsymbol{\omega}_{1}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\|\boldsymbol{X} \cdot \boldsymbol{\omega}\|^{2}\right\}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\boldsymbol{\omega}^{\top} \boldsymbol{X}^{\top} \boldsymbol{X} \boldsymbol{\omega}\right\}
$$




Second Compoment is $\boldsymbol{z}_{2}=\boldsymbol{X} \boldsymbol{\omega}_{2}$ where

$$
\boldsymbol{\omega}_{2}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\left\|\widetilde{\boldsymbol{X}}^{(1)} \cdot \boldsymbol{\omega}\right\|^{2}\right\}
$$


with $\widetilde{\boldsymbol{X}}^{(1)}=\boldsymbol{X}-\underbrace{\boldsymbol{X} \omega_{1}}_{z_{1}} \omega_{1}^{\top}$.

## Reducing Dimension with PCA

A regression on (the $d$ ) principal components, $y=\boldsymbol{z}^{\top} \boldsymbol{b}+\boldsymbol{\eta}$ could be an interesting idea, unfortunatley, principal components have no reason to be correlated with $y$. First compoment was $\boldsymbol{z}_{1}=\boldsymbol{X} \boldsymbol{\omega}_{1}$ where

$$
\boldsymbol{\omega}_{1}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\|\boldsymbol{X} \cdot \boldsymbol{\omega}\|^{2}\right\}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\boldsymbol{\omega}^{\top} \boldsymbol{X}^{\top} \boldsymbol{X} \boldsymbol{\omega}\right\}
$$

It is a non-supervised technique.
Instead, use partial least squares, introduced in Wold (1966). First compoment is $\boldsymbol{z}_{1}=\boldsymbol{X} \boldsymbol{\omega}_{1}$ where

$$
\boldsymbol{\omega}_{1}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\{<\boldsymbol{y}, \boldsymbol{X} \cdot \boldsymbol{\omega}>\}=\underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}}\left\{\boldsymbol{\omega}^{\top} \boldsymbol{X}^{\top} \boldsymbol{y} \boldsymbol{y}^{\top} \boldsymbol{X} \boldsymbol{\omega}\right\}
$$

(etc.)

## Instrumental Variables

Consider some instrumental variable model, $y_{i}=\boldsymbol{x}_{i}^{\boldsymbol{\top}} \boldsymbol{\beta}+\varepsilon_{i}$ such that

$$
\mathbb{E}\left[Y_{i} \mid \boldsymbol{Z}\right]=\mathbb{E}\left[\boldsymbol{X}_{i} \mid \boldsymbol{Z}\right]^{\top} \boldsymbol{\beta}+\mathbb{E}\left[\varepsilon_{i} \mid \boldsymbol{Z}\right]
$$

The estimator of $\boldsymbol{\beta}$ is

$$
\widehat{\boldsymbol{\beta}}_{\mathrm{IV}}=\left[\boldsymbol{Z}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{Z}^{\top} \boldsymbol{y}
$$

If $\operatorname{dim}(\boldsymbol{Z})>\operatorname{dim}(\boldsymbol{X})$ use the Generalized Method of Moments,

$$
\widehat{\boldsymbol{\beta}}_{\mathrm{GMM}}=\left[\boldsymbol{X}^{\top} \boldsymbol{\Pi}_{\boldsymbol{Z}} \boldsymbol{X}\right]^{-1} \boldsymbol{X}^{\top} \boldsymbol{\Pi}_{\boldsymbol{Z}} \boldsymbol{y} \text { with } \boldsymbol{\Pi}_{\boldsymbol{Z}}=\boldsymbol{Z}\left[\boldsymbol{Z}^{\top} \boldsymbol{Z}\right]^{-1} \boldsymbol{Z}^{\top}
$$

## Instrumental Variables

Consider a standard two step procedure

1) regress colums of $\boldsymbol{X}$ on $\boldsymbol{Z}, \boldsymbol{X}=\boldsymbol{Z} \boldsymbol{\alpha}+\boldsymbol{\eta}$, and derive predictions $\widehat{\boldsymbol{X}}=\boldsymbol{\Pi}_{\boldsymbol{Z}} \boldsymbol{X}$
2) regress $Y$ on $\widehat{\boldsymbol{X}}, y_{i}=\widehat{\boldsymbol{x}}_{\boldsymbol{i}}^{\top} \boldsymbol{\beta}+\varepsilon_{i}$, i.e.

$$
\widehat{\boldsymbol{\beta}}_{\mathrm{IV}}=\left[\boldsymbol{Z}^{\top} \boldsymbol{X}\right]^{-1} \boldsymbol{Z}^{\top} \boldsymbol{y}
$$

See Angrist \& Krueger (1991) with 3 up to 1530 instruments : 12 instruments seem to contain all necessary information.

Use LASSO to select necessary instruments, see Belloni, Chernozhukov \& Hansen (2010)

## Take Away Conclusion

Big data mythology

- $n \rightarrow \infty: 0 / 1$ law, everything is simplified (either true or false)
- $p \rightarrow \infty$ : higher algorithmic complexity, need variable selection tools

Econometrics vs. Machine Learning

- probabilistic interpretation of econometric models (unfortunately sometimes misleading, e.g. $p$-value) can deal with non-i.id data (time series, panel, etc)
- machine learning is about predictive modeling and generalization algorithmic tools, based on bootstrap (sampling and sub-sampling), cross-validation, variable selection, nonlinearities, cross effects, etc

Importance of visualization techniques (forgotten in econometrics publications)

