Stochastic Gradient Descent and (Feedforward) Neural Networks

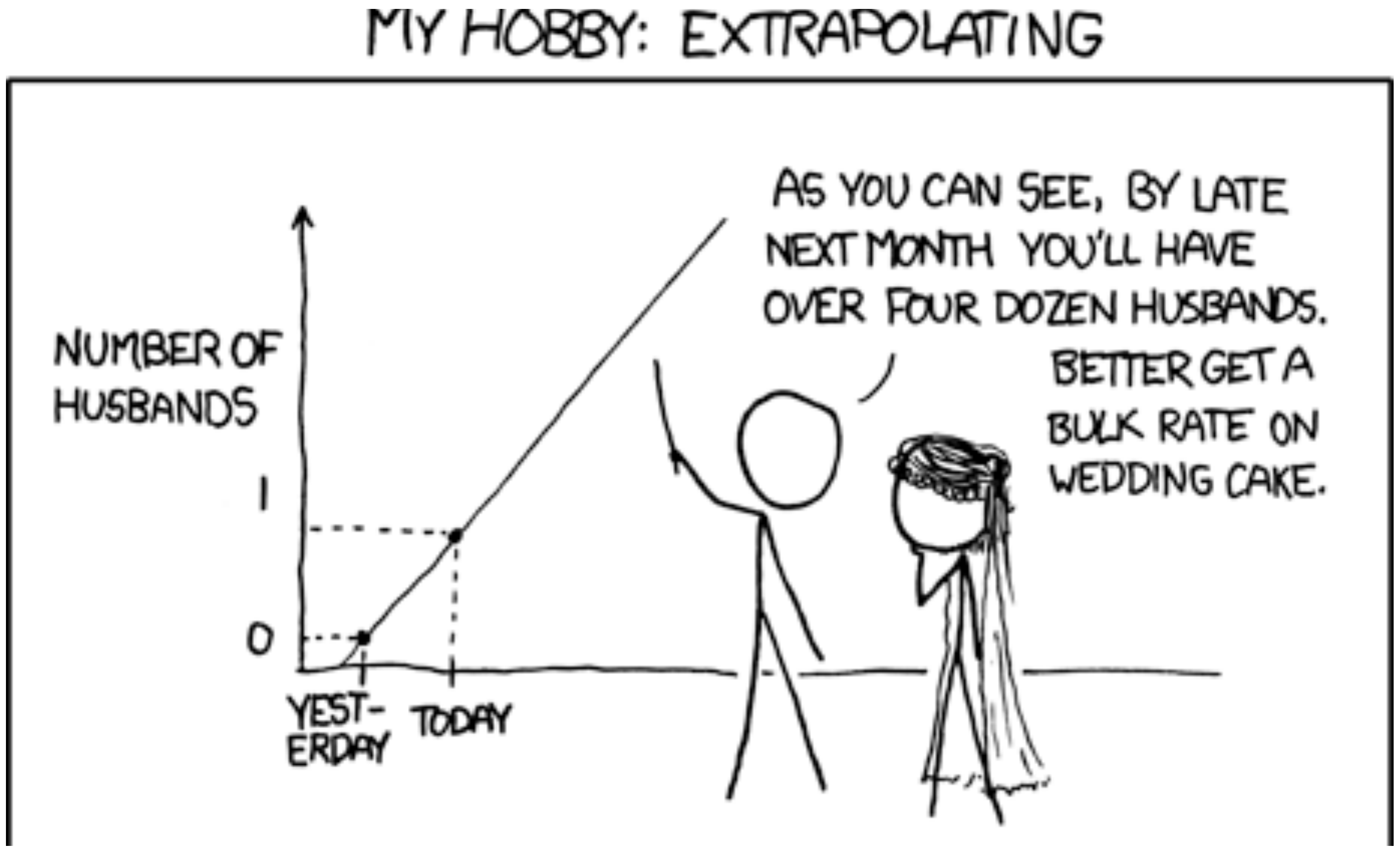
(Recap) Linear Regression

- Studied extensively and have well-developed theory (variable selection methods, extensions for dealing with correlated data, evaluation of results,...)

  Model: $E(y \mid \mathbf{x}) = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k$ + i.i.d. Gaussian error term

- Evaluating the coefficients
  - consider standard errors
  - Consider coefficients if both x and y's were normalized
  - Doing significance test to see if each term should be dropped.
  - Many predictors? Better to do forward search…

Knowing Scope of Models


MY HOBBY: EXTRAPOLATING
NUMBER OF HUSBANDS
1
0
YEST-ERDAY
TODAY
AS YOU CAN SEE, BY LATE NEXT MONTH YOU'LL HAVE OVER FOUR DOZEN HUSBANDS. BETTER GET A BULK RATE ON WEDDING CAKE.

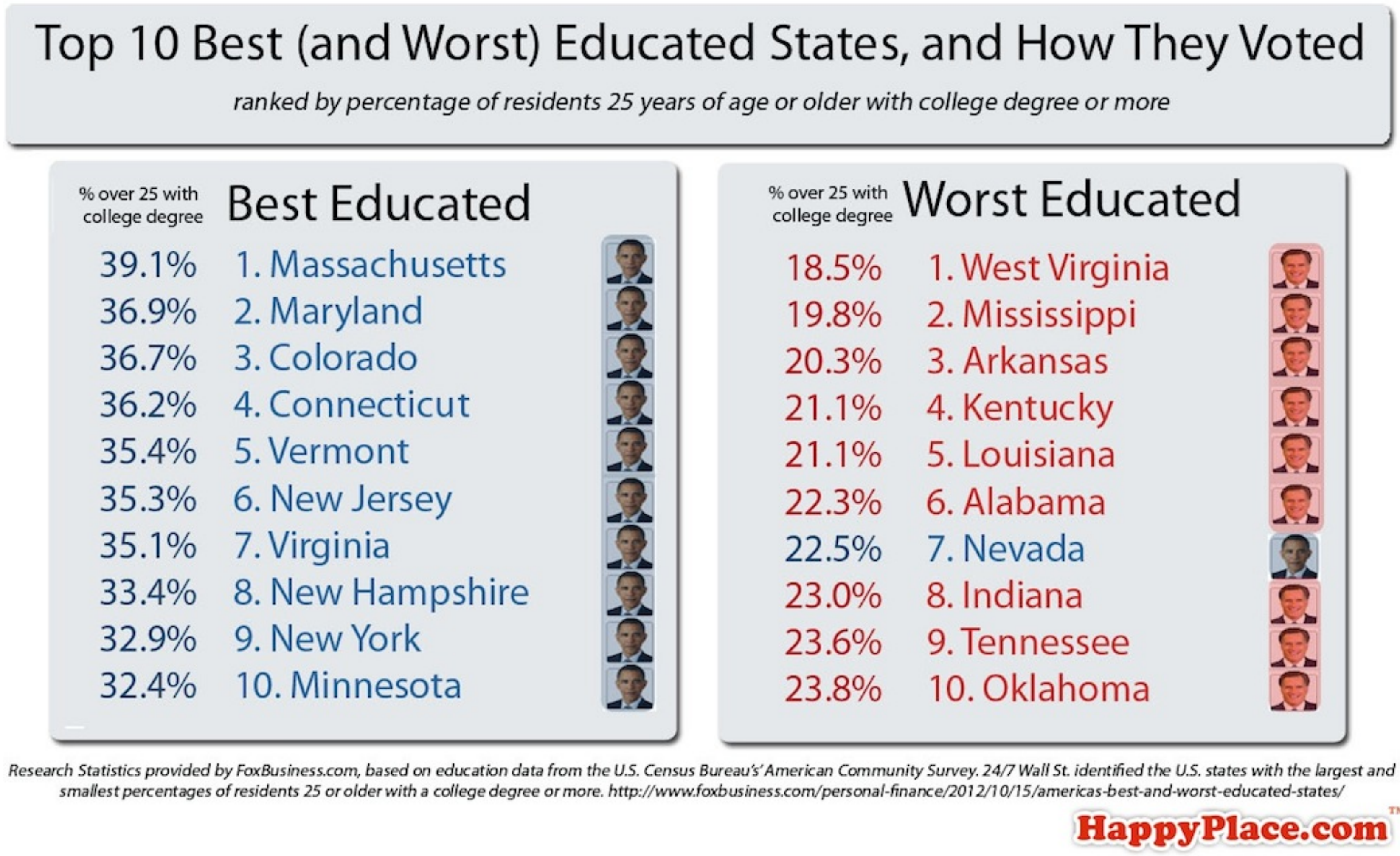
Beyond linear Regression

- linear regression
- almost linear methods
  - generalized linear models
  - Multi-level models
  - additive models
  - piecewise linear (e.g. CART); locally linear regression, ….

- nonlinear models
  - linear in fixed transform (“phi”) space (Fourier, Gabor, polynomial…)
  - general nonlinear forms (basis functions are adaptive as well)
    - e.g. feedforward neural networks (MLP, RBF,…)
    - MLP, RBFs, Polynomials are all universal approximators

Correlation vs. Causation

- Though it may still be actionable



Top 10 Best (and Worst) Educated States, and How They Voted

ranked by percentage of residents 25 years of age or older with college degree or more

% over 25 with college degree	Best Educated	
39.1%	1. Massachusetts	🟦
36.9%	2. Maryland	🟦
36.7%	3. Colorado	🟦
36.2%	4. Connecticut	🟦
35.4%	5. Vermont	🟦
35.3%	6. New Jersey	🟦
35.1%	7. Virginia	🟦
33.4%	8. New Hampshire	🟦
32.9%	9. New York	🟦
32.4%	10. Minnesota	🟦

% over 25 with college degree	Worst Educated	
18.5%	1. West Virginia	🟥
19.8%	2. Mississippi	🟥
20.3%	3. Arkansas	🟥
21.1%	4. Kentucky	🟥
21.1%	5. Louisiana	🟥
22.3%	6. Alabama	🟥
22.5%	7. Nevada	🟦
23.0%	8. Indiana	🟥
23.6%	9. Tennessee	🟥
23.8%	10. Oklahoma	🟥

Research Statistics provided by FoxBusiness.com, based on education data from the U.S. Census Bureau's' American Community Survey. 24/7 Wall St. identified the U.S. states with the largest and smallest percentages of residents 25 or older with a college degree or more. http://www.foxbusiness.com/personal-finance/2012/10/15/americas-best-and-worst-educated-states/

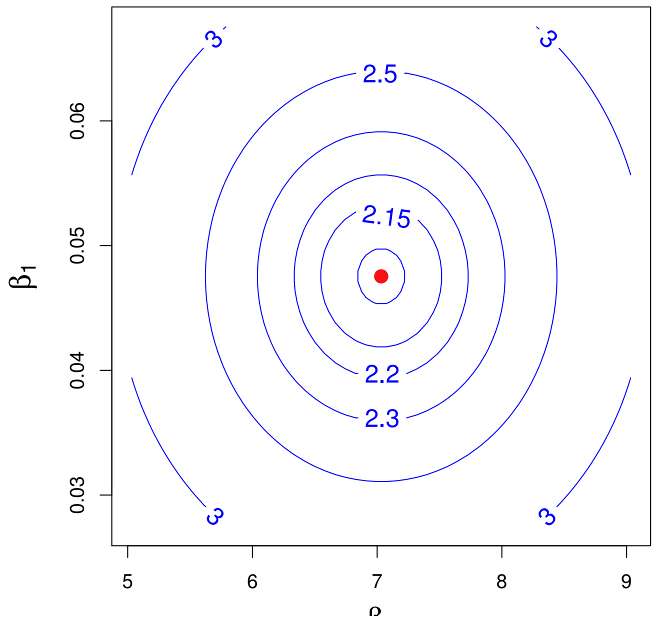
HappyPlace.com™

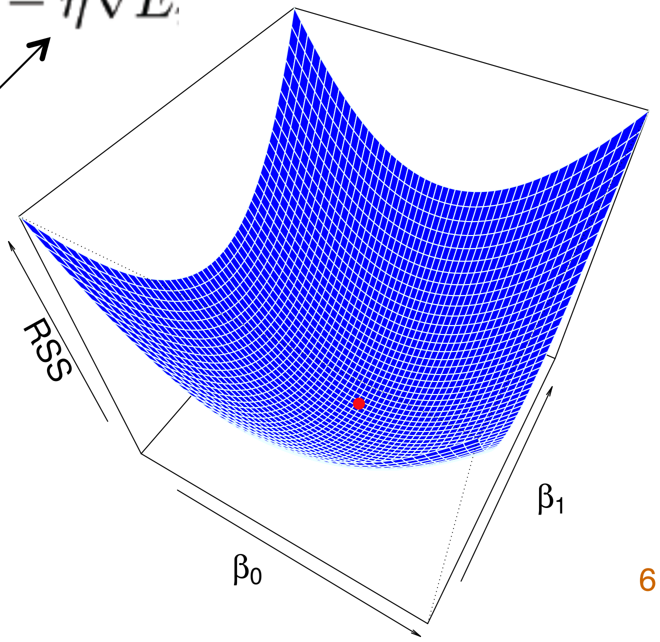
Gradient Descent for Linear Models

- **See (very introductory) Coursera Lectures by Andrew Ng, and Bishop Ch 5.1, 5.2**
- The cost function $E(\mathbf{w})$ is quadratic in $\mathbf{w}$
  - $E(\mathbf{w}) = \text{SSE}(\mathbf{w}) = \text{SSE}(\mathbf{w}^*) + (\mathbf{w}-\mathbf{w}^*)^T\mathbf{Q}(\mathbf{w}-\mathbf{w}^*)$
    - $\mathbf{w}^*$ is the optimum solution, and $\mathbf{Q}$ a positive definite matrix.
    - SSE = sum of squared error (also called Residual Sum Squares or RSS)
    - Hence error surface is convex in weight space, so weights can be obtained by doing gradient descent **(incrementally moving down the cost surface in weight space)**

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta\nabla E$$

Learning rate





Learning Rate

- Learning rate η(t) is crucial
  - Too low, too slow; too high, unstable
- True gradient descent is batch algorithm, slow (but sure)
- "on-line" version (**stochastic gradient descent or SGD**): replace true gradient by "instantaneous" gradient, that reduces error only on the new instance (pun intended!)

$$\begin{aligned}\mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} - \eta \nabla E_n \\ &= \mathbf{w}^{(\tau)} + \eta(t_n - \mathbf{w}^{(\tau)\mathrm{T}}\phi(\mathbf{x}_n))\phi(\mathbf{x}_n).\end{aligned}$$

- This is known as the *least-mean-squares (LMS) algorithm*
  - Note: Data items considered one at a time (a.k.a. online learning)

Stokhos = "to aim"

Sequential Learning with SGD

- Learning rate: too small → too slow
  - Too large → oscillatory, or may even diverge
- Should η be fixed or adaptive (second order methods)?
- Is convergence needed or not?
  - Non-stationary? May not want to converge!
  - If convergence is desired, then η should decrease with time.
  - * Robbins-Monroe Sequence is adequate (e.g. $\eta(t) = 1/t$)
    - Sum of absolute values (of sequence of η values) is unbounded
    - Sum of squared values is finite
    - Values in decreasing sequence

Why SGD?

Better for large data sets

+ Often faster than batch gradient descent

    Can do "mini-batches" as a practical trade-off

+ Less prone to local minima, so often applied to complex models (and correspondingly complex error surfaces)

+ useful to scale inputs to help find learning rate (usually fixed)

+ works for non-stationary environments as well as online settings

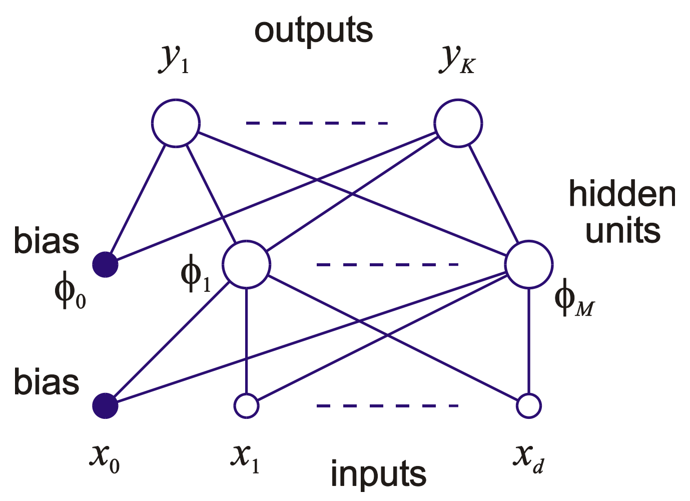
Also used for more complex error surfaces, though many second-order methods, that also consider the Hessian (matrix of curvatures) in addition to the Jacobian, or vector of slopes, exist.

Active research/application area right now!

https://www.ipam.ucla.edu/programs/workshops/stochastic-gradient-methods/

Multi-Layered Perceptrons (MLP) (most popular neural network)

- 1 hidden layer → 2 layered network.
- Choice of activation functions:
- Hidden layer: tanh/sigmoid
  - Why not LTU
- Output layer: linear / sigmoid or softmax
-



Typical MLP for Regression
(2 layers of adaptive weights):

$$y_k(\mathbf{x}, \mathbf{w}) = \sum_{j=1}^{M} w_{kj}^{(2)} \tanh\left(\sum_i w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}$$

Design Parameters to be Aware about

- # of hidden units/nodes
  - model complexity
- # of epochs/iterations
  - how long do you train: best is use a cross-validation set to decide when to stop
- Activation function
  - typically tanh or logistic, a.k.a. sigmoid
- Learning rate (SGD is used to update weights)
  - Speed o

- Momentum: if you want a second order gradient descent methods, use some momentum.

(Multi-path) Chain Rule from Calculus*

$$\begin{tikzcd}
 & z & \\
y_1 \arrow[ur, "\frac{\partial z}{\partial y_1}"] & & y_2 \arrow[ul, "\frac{\partial z}{\partial y_2}"'] \\
 & x \arrow[ul, "\frac{\partial y_1}{\partial x}"] \arrow[ur, "\frac{\partial y_2}{\partial x}"'] &
\end{tikzcd}$$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

Weight Update through Error Back-propagation*

Takeaway: weights are updated through (online) SGD

- Derived from chain rule for partial derivatives
- Three stages:

1. Evaluate an “error signal” at the output units with net input a_k

$$\delta_k = \frac{\partial E_n}{\partial a_k}$$

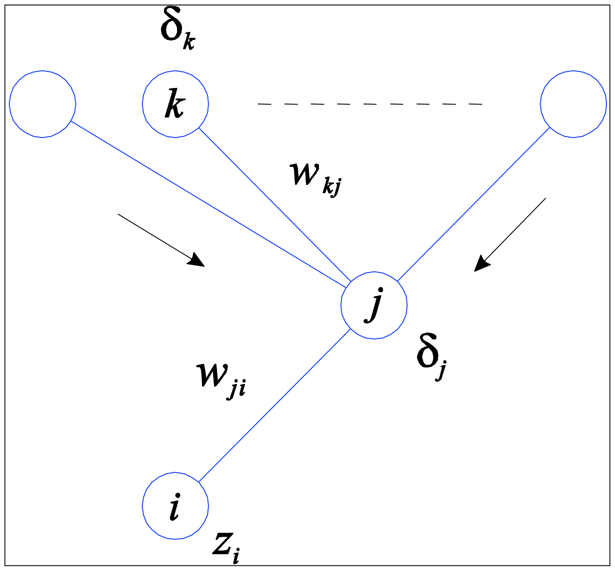
2. Propagate the signal backwards through the network

$$\delta_j = g'(a_j) \sum_k w_{kj} \delta_k$$

3. Evaluate derivatives

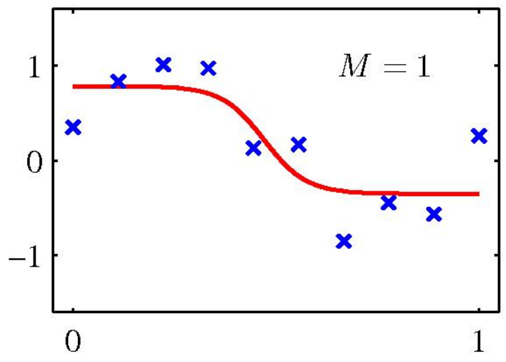
$$\frac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$$

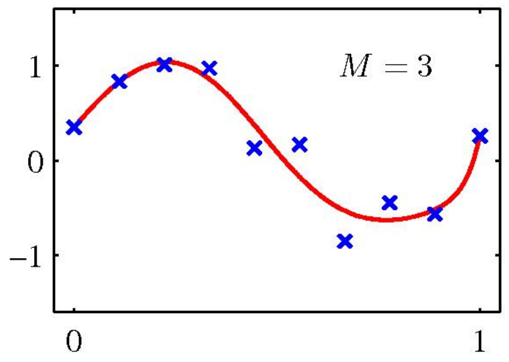
4. Use this for SGD

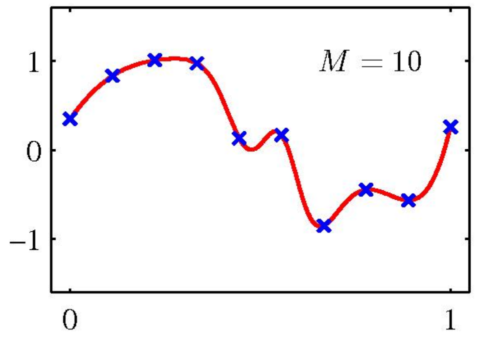


Model Complexity for MLP

- complexity related to # of hidden units AND amount of training (number of passes or epochs through the data)





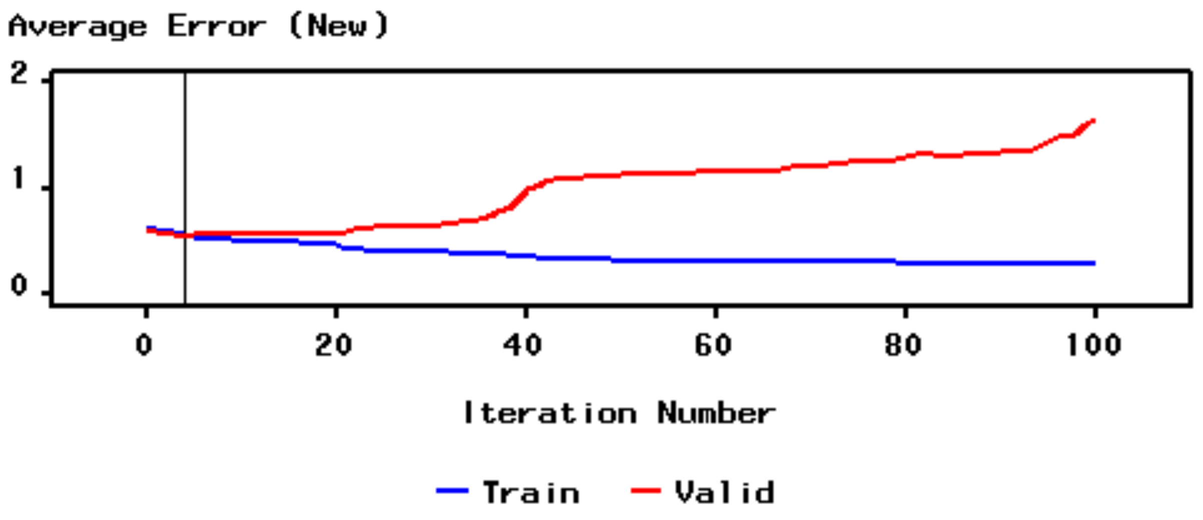


With less training M=10 solution looks like M < 10…

Adjusting Complexity

– "effective # of parameters" increases with # of epochs !!
  - Select adequately powerful model
  - while training, monitor performance using validation set
  - **stop training** when error on validation set reaches a minimum

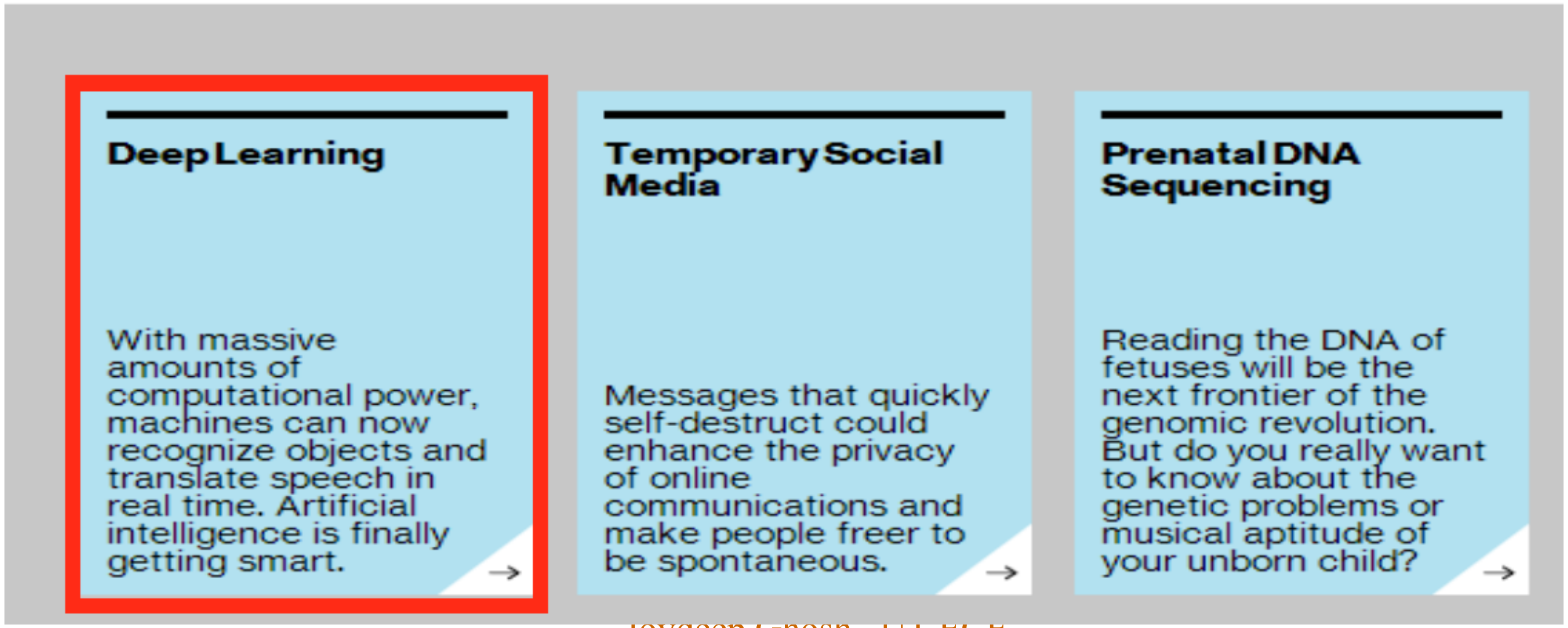
  - SAS fig.



Deep Learning

- Amazing improvements in speech recognition, NLP, recognizing objects in images,…

MIT Technology Review
10 BREAKTHROUGH TECHNOLOGIES 2013


Deep Learning

With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart. →

Temporary Social Media

Messages that quickly self-destruct could enhance the privacy of online communications and make people freer to be spontaneous. →

Prenatal DNA Sequencing

Reading the DNA of fetuses will be the next frontier of the genomic revolution. But do you really want to know about the genetic problems or musical aptitude of your unborn child? →

Going Deep

See tutorial at: http://www.iro.umontreal.ca/~bengioy/talks/mlss-austin.pdf

From Facebook's Deepface paper
https://facebook.com//download/233199633549733/deepface.pdf
Our method reaches an accuracy of 97.35% on the Labeled Faces in the Wild (LFW) dataset, reducing the error of the current state of the art by more than 27%, closely approaching human-level performance.

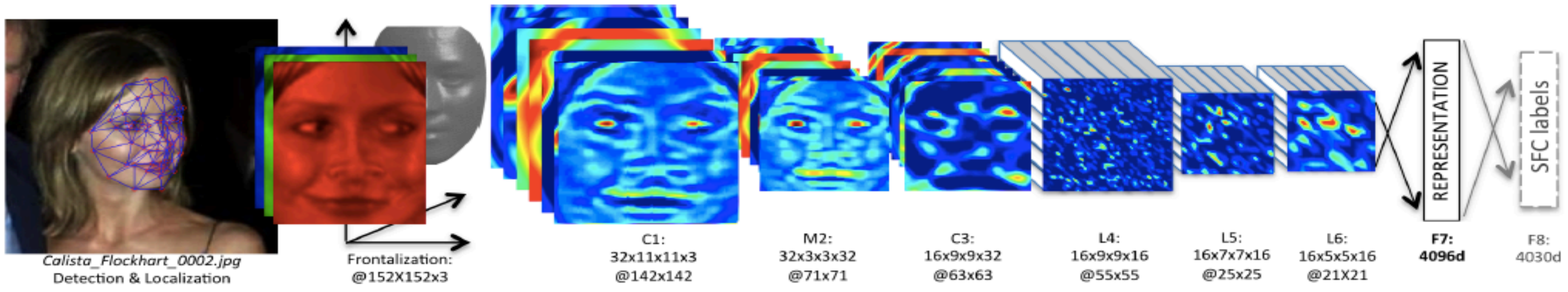


Figure 2. **Outline of the *DeepFace* architecture.** A front-end of a single convolution-pooling-convolution filtering on the rectified input, followed by three locally-connected layers and two fully-connected layers. Colors illustrate outputs for each layer. The net includes more than 120 million parameters, where more than 95% come from the local and fully connected layers.

Multilevel Models (MLM)

- “Multilevel modeling is a generalization of generalized linear modeling” (Gelman, 2005)
- Multilevel model = Hierarchical model = Mixed Effect model = …
- “Level” in multilevel refers to the hierarchy of parameters
  - Usually refers to a hierarchy of groupings of the individual entities

When do we use, and Why do we need it?

- Example: We want to study alcohol abuse among young people (Dominici, 2005)
  - A person is a member of a family, and a resident of a state
  - Level 1 (person): person’s ability to metabolize alcohol
  - Level 2 (family): alcohol abuse in the family
  - Level 3 (state): state laws
- Multilevel modeling is useful when
  - Not enough data for lowest level models while higher level models are too coarse
  - or desire to get similar results for individuals within a group
- MLM models entities at the lowest level, but “borrows strength from” higher levels

When does it make a difference?

Classical regression vs. Multilevel modeling

- When there is very little group-level variation, multilevel modeling reduces to classical regression with no group indicators
- When group-level coefficients vary greatly, multilevel modeling reduces to classical regression with group indicators (group dummy codes)

So advantageous "in-between", or when domain knowledge or business process dictates that certain parameters be softly "tied together"

Alcohol Use among Adolescents

- Three years of longitudinal data
- 82 adolescents, beginning at age 14
- Covariates:
  - COA: an indicator variable whether the adolescent is a child of alcoholic parent
  - PEER: 8-point scale that shows the proportion of their friends who drink alcohol
  - time: 0, 1, 2 (three years)
- 2 Levels: individuals (i=1,…82), and whole group, indexed by i=0

Proposed Multilevel Model

$$\begin{aligned}
y_{it} &= \beta_{0i} + \beta_p p_{it} + \beta_c c_{it} + \beta_{1i} t + \epsilon_{it} \\
\beta_{0i} &= \beta_{00} + b_{0i} \\
\beta_{1i} &= \beta_{10} + b_{1i} \\
(b_{0i}, b_{1i} & \text{ are noise terms (called random effects; to contrast with} \\
& \beta\text{s, which are "fixed effects")} \\
y_{it} : & \text{ Alcohol use} \\
c_{it} : & \text{ COA} \\
p_{it} : & \text{ PEER} \\
t : & \text{ time}
\end{aligned}$$

What is the corresponding MLR?

Statistical Details*

$$\boxed{\begin{aligned} \mathbf{y}_i &= \mathbf{X}_i\boldsymbol{\beta} + \mathbf{Z}_i\mathbf{b}_i + \boldsymbol{\epsilon}_i \\ \mathbf{b}_i &\sim \mathrm{N}(0, \sigma^2\mathbf{D}) \\ \boldsymbol{\epsilon}_i &\sim \mathrm{N}(0, \sigma^2\mathbf{I}) \end{aligned}}$$

$$\begin{aligned} &L(\boldsymbol{\beta}, \mathbf{D}, \sigma^2 \mid \mathbf{Y}) \\ &= \prod p(\mathbf{y}_i \mid \boldsymbol{\beta}, \mathbf{D}, \sigma^2) \\ &= \prod \int p(\mathbf{y}_i \mid \mathbf{b}_i, \boldsymbol{\beta}, \sigma^2) p(\mathbf{b}_i \mid \mathbf{D}, \sigma^2) d\mathbf{b}_i \\ &= \prod \frac{1}{\sqrt{(2\pi\sigma^2)^{n_i}|\mathbf{D}|}} \int \frac{\exp \frac{-1}{2\sigma^2}(\|\mathbf{y}_i - \mathbf{X}_i\boldsymbol{\beta} - \mathbf{Z}_i\mathbf{b}_i\| + \mathbf{b}_i^\top \mathbf{D}^{-1}\mathbf{b}_i)}{(2\pi\sigma^2)^{q/2}} d\mathbf{b}_i \end{aligned}$$

Computational Details*

Takeaway: There are several ways of estimating the parameters (given as an option in the R code), all are somewhat involved compared to MLR.

- Maximum Likelihood Estimation
  - with respect to all the parameters
  - EM iterations

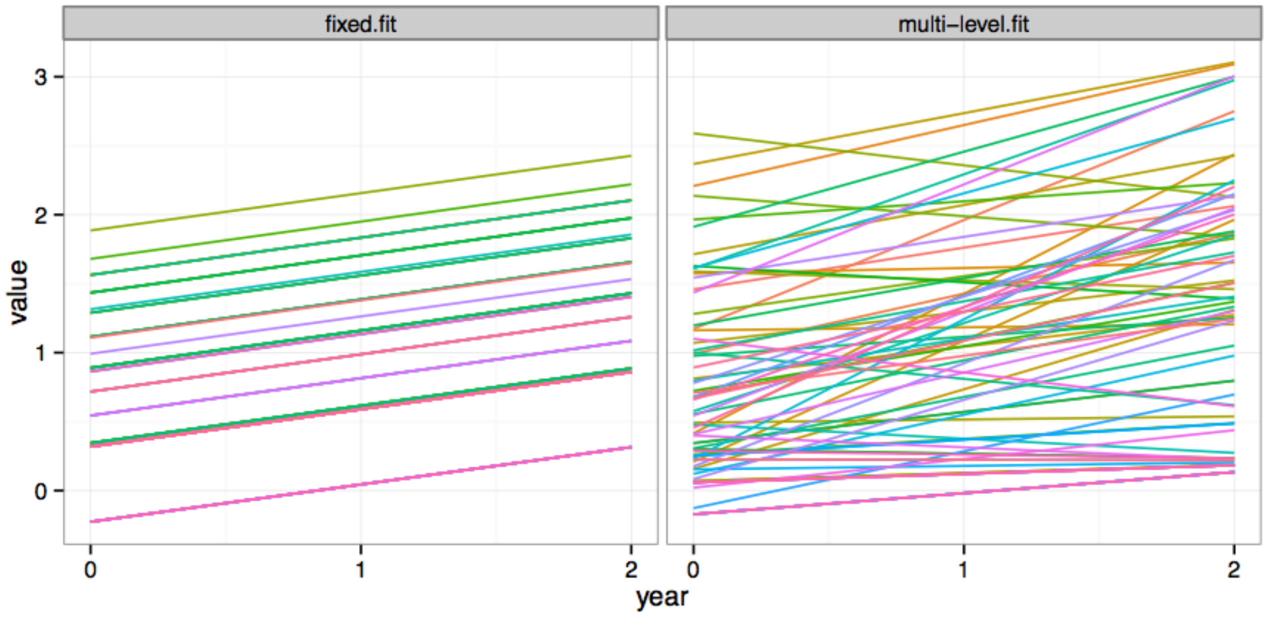
While My MCMC Gently Samples

- Restricted Maximum Likelihood Estimation
  - focusing only on D (random-effect covariance) (Harville, 1976)
  - EM iterations
- Bayesian Posterior Estimation
  - Gibbs sampling using R and Bugs (Gelman and Hill, 2007)

In R, using package(nlme)

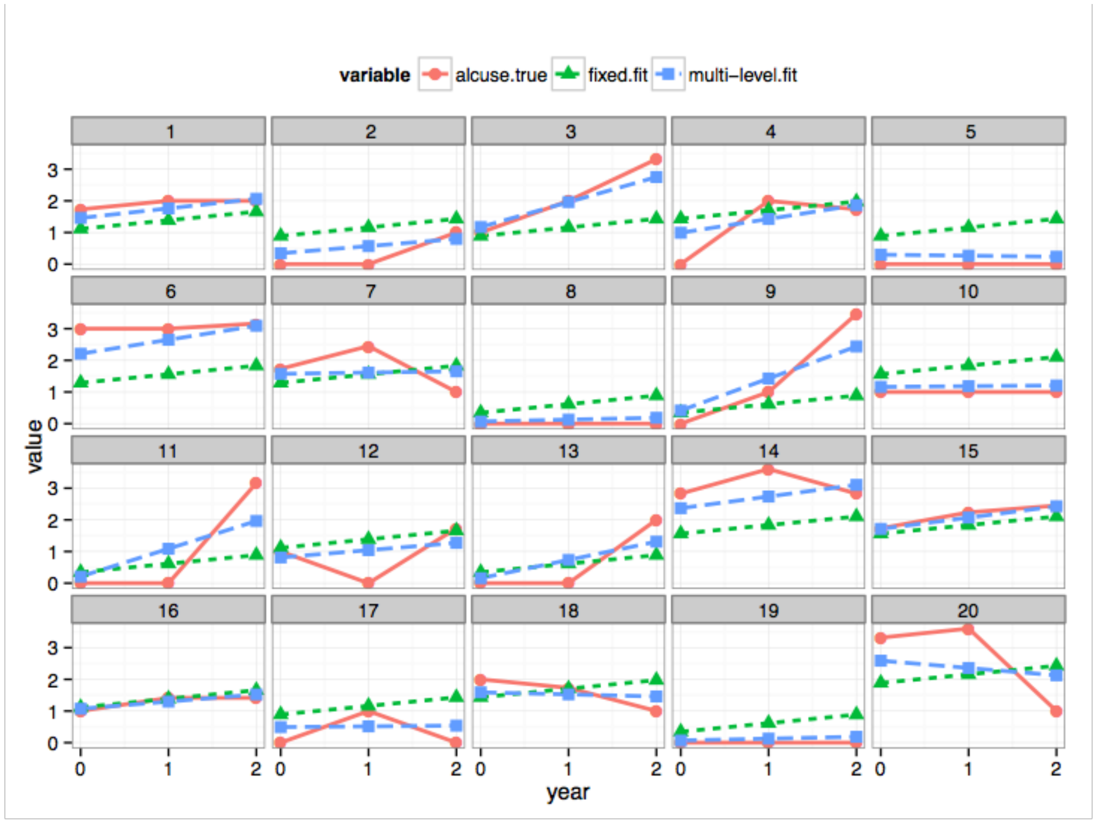
```
> model.e <- lme(alcuse ~ coa+peer+time , data=df, random= ~ time | id, method="REML")
> summary(model.e)
Linear mixed-effects model fit by REML
 Data: df
      AIC      BIC    logLik
  619.7211 647.6326 -301.8606

Random effects:
 Formula: ~time | id
 Structure: General positive-definite, Log-Cholesky parametrization
            StdDev    Corr
(Intercept) 0.5119870 (Intr)
time        0.3938927 -0.075
Residual    0.5807686

Fixed effects: alcuse ~ coa + peer + time
                 Value  Std.Error  DF   t-value p-value
(Intercept) -0.2263521 0.14036356 163 -1.612613  0.1088
coa          0.5711970 0.14897721  79  3.834123  0.0003
peer         0.6092227 0.10226024  79  5.957572  0.0000
time         0.2706514 0.06283908 163  4.307056  0.0000
 Correlation:
     (Intr) coa    peer
coa  -0.359
peer -0.664 -0.162
time -0.254  0.000  0.000

Standardized Within-Group Residuals:
       Min         Q1        Med         Q3        Max
-2.5999504 -0.3984809 -0.1047824  0.3732800  2.3604876

Number of Observations: 246
Number of Groups: 82
```

Alcohol Use Example (continued)



[Alcohol use among adolescents] Original data, and fitted curves from multilevel and classical regression. The multilevel model captures the individual-differences on the changes of alcohol use.

Alcohol Use Example (continued)



[Alcohol use among adolescents] Original data, and fitted curves from multilevel and classical regression. The multilevel model captures the individual-differences on the changes of alcohol use.

References for MLM

- (nlme in R) http://cran.r-project.org/web/packages/nlme/nlme.pdf
- (lme4 in R) http://cran.r-project.org/web/packages/lme4/lme4.pdf
- (Dominici, 2005) http://www.biostat.jhsph.edu/bstcourse/bio607/
- (Bates and Pinheiro) http://www.stat.bell-labs.com/NLME/CompMulti.pdf
- (Papers on multilevel modeling) http://www.ats.ucla.edu/stat/papers/ mlmpapers.htm
- (Gelman, 2005) Gelman, Andrew. "Multilevel (hierarchical) modeling: what it can and cannot do." *Technometrics* 48.3 (2006). http://www.cs.berkeley.edu/~russell/classes/cs294/f05/papers/gelman-2005.pdf

- PYTHON implementation: part of PyMC3
  - https://pymc-devs.github.io/pymc3/GLM-hierarchical/
  - While My MCMC Gently Samples

So which method should I choose?

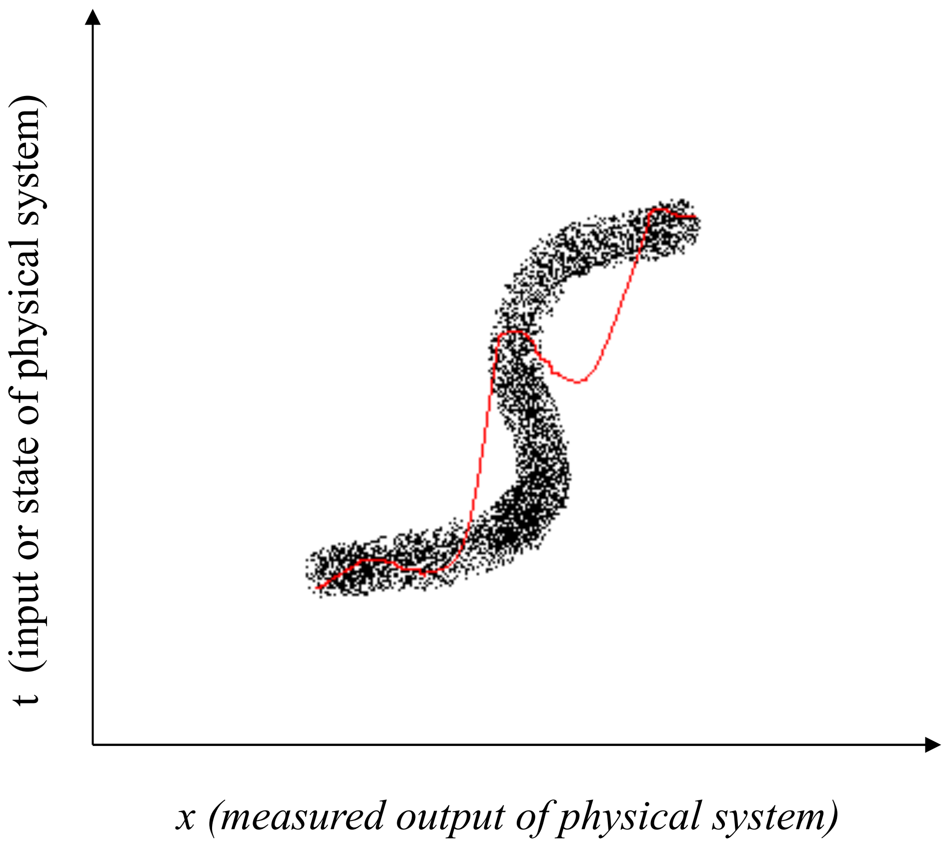
- Depends on type, complexity of problem; data size
  - (i) try linear regression first
    - Explore data; Study residues
    - do feature selection/transformation if needed
    - If robustness is needed, try "rlm" (R package), or use SVR.
  - (ii) Now try a set of powerful but not so interpretable models (MLP etc)
    - (estimate complexity of fit using a few trial runs)
  - How much is the gap between (i) and (ii)?
  - Consider Decision tree based regression if interpretation is important or a piecewise constant answer is more "actionable"

- Still lacking? try ensemble approaches
  specially gbdt, which also rank orders the features.

Caution: Modeling **Inverse** Problems

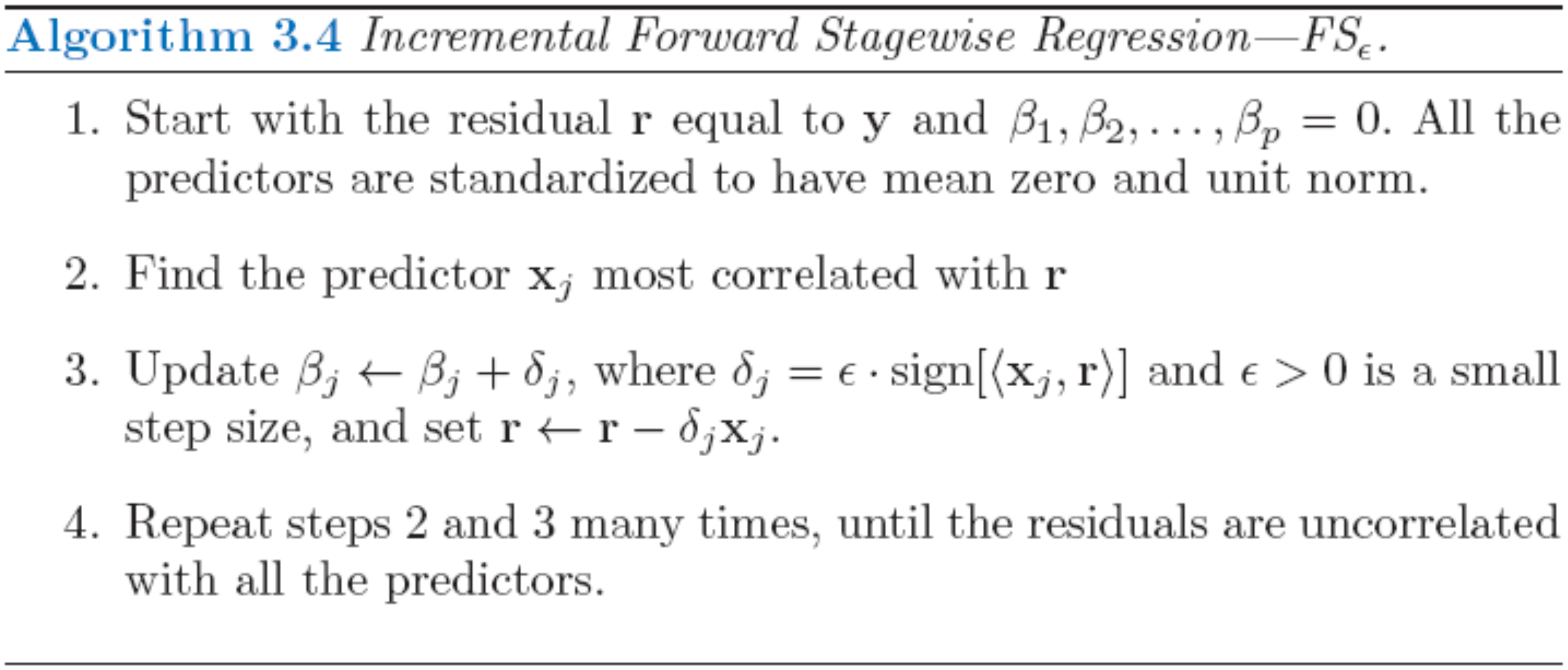
- Forward problem reasonably characterized by a function, but not the reverse problem
- t is not h(**x**) + (zero-mean, unimodal) noise

  So Least squares solution will bomb
- Solution: model joint pdf
  - Or piecewise models



Extras

Incremental Forward Stagewise Regression (HTF 3.8)



Algorithm 3.4 *Incremental Forward Stagewise Regression—FS_ϵ.*

1. Start with the residual $\mathbf{r}$ equal to $\mathbf{y}$ and $\beta_1, \beta_2, \ldots, \beta_p = 0$. All the predictors are standardized to have mean zero and unit norm.
2. Find the predictor $\mathbf{x}_j$ most correlated with $\mathbf{r}$
3. Update $\beta_j \leftarrow \beta_j + \delta_j$, where $\delta_j = \epsilon \cdot \text{sign}[\langle \mathbf{x}_j, \mathbf{r} \rangle]$ and $\epsilon > 0$ is a small step size, and set $\mathbf{r} \leftarrow \mathbf{r} - \delta_j \mathbf{x}_j$.
4. Repeat steps 2 and 3 many times, until the residuals are uncorrelated with all the predictors.

HTF, pg 87

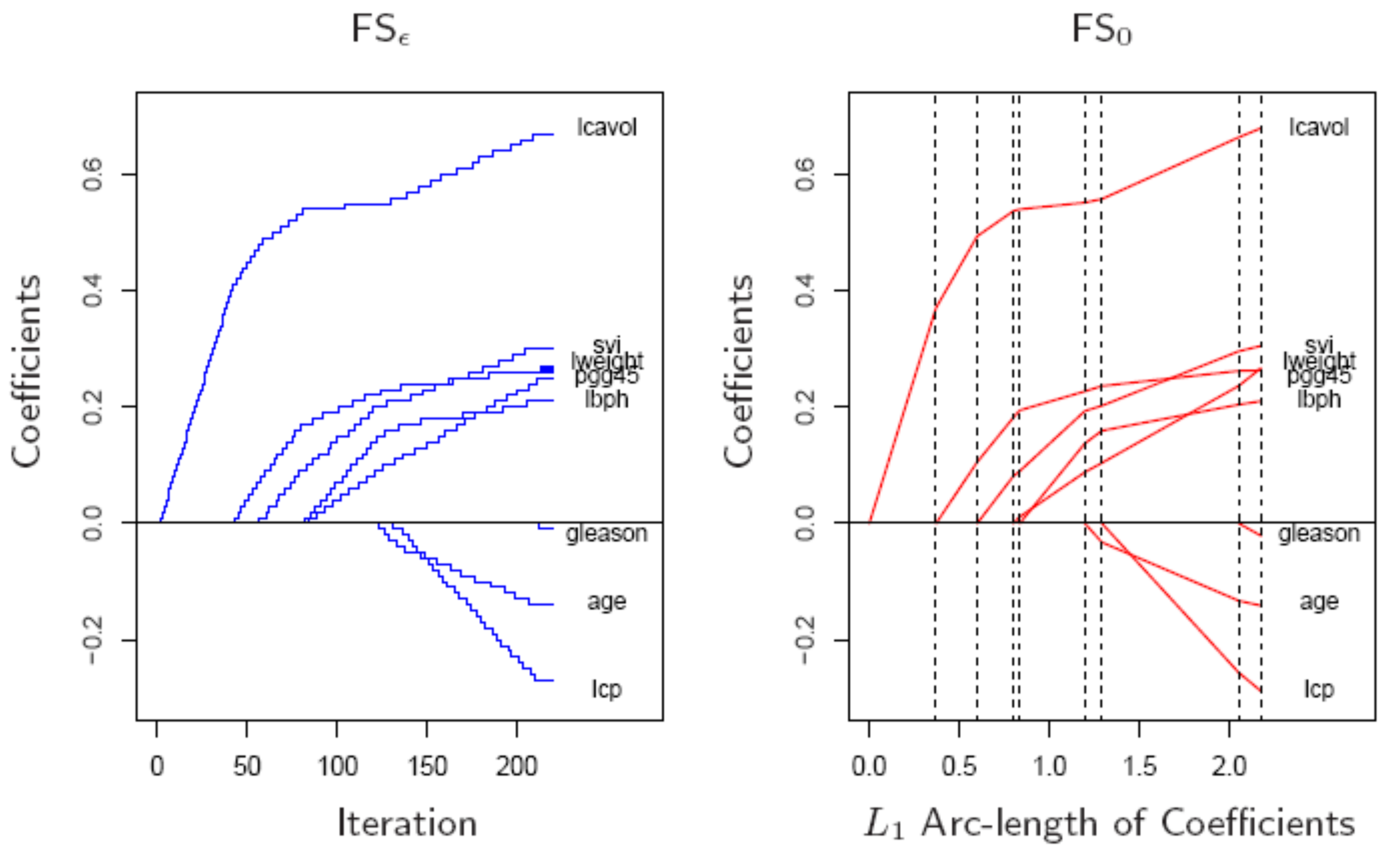
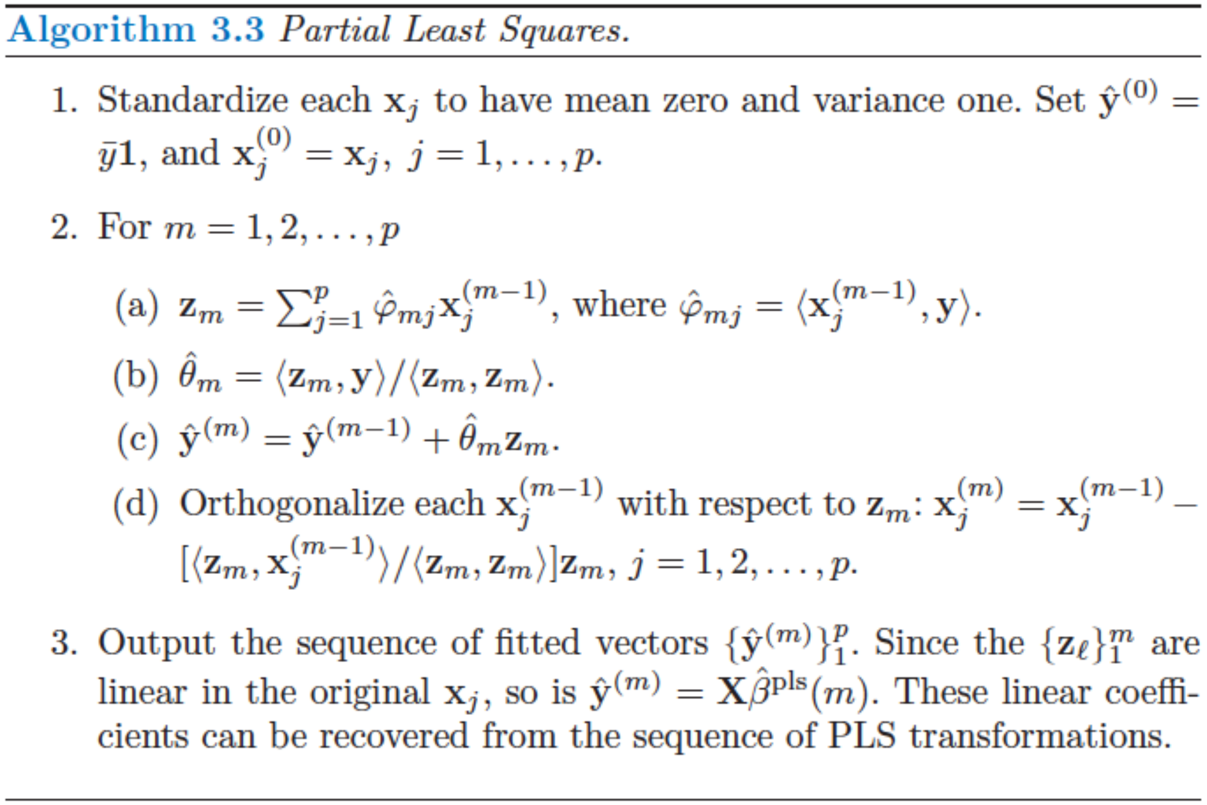


FIGURE 3.19. *Coefficient profiles for the prostate data. The left panel shows incremental forward stagewise regression with step size $\epsilon = 0.01$. The right panel shows the infinitesimal version FS_0 obtained letting $\epsilon \to 0$. This profile was fit by the modification 3.2b to the LAR Algorithm 3.2. In this example the FS_0 profiles are monotone, and hence identical to those of lasso and LAR.*

Regression on Derived Input Projections (HTF 3.5)

- PCR: Principal Component Regression
- PLS: Partial Least Squares

pls package contains both. Typically their effect is similar to ridge regression, but shrinking of coefficients not so smooth



Algorithm 3.3 *Partial Least Squares.*

```
1. Standardize each $\mathbf{x}_j$ to have mean zero and variance one. Set $\hat{\mathbf{y}}^{(0)} = \bar{y}\mathbf{1}$, and $\mathbf{x}_j^{(0)} = \mathbf{x}_j,\ j = 1, \ldots, p$.

2. For $m = 1, 2, \ldots, p$

   (a) $\mathbf{z}_m = \sum_{j=1}^{p} \hat{\varphi}_{mj}\mathbf{x}_j^{(m-1)}$, where $\hat{\varphi}_{mj} = \langle \mathbf{x}_j^{(m-1)}, \mathbf{y} \rangle$.
   (b) $\hat{\theta}_m = \langle \mathbf{z}_m, \mathbf{y} \rangle / \langle \mathbf{z}_m, \mathbf{z}_m \rangle$.
   (c) $\hat{\mathbf{y}}^{(m)} = \hat{\mathbf{y}}^{(m-1)} + \hat{\theta}_m \mathbf{z}_m$.
   (d) Orthogonalize each $\mathbf{x}_j^{(m-1)}$ with respect to $\mathbf{z}_m$: $\mathbf{x}_j^{(m)} = \mathbf{x}_j^{(m-1)} - [\langle \mathbf{z}_m, \mathbf{x}_j^{(m-1)} \rangle / \langle \mathbf{z}_m, \mathbf{z}_m \rangle]\mathbf{z}_m,\ j = 1, 2, \ldots, p$.

3. Output the sequence of fitted vectors $\{\hat{\mathbf{y}}^{(m)}\}_1^p$. Since the $\{\mathbf{z}_\ell\}_1^m$ are linear in the original $\mathbf{x}_j$, so is $\hat{\mathbf{y}}^{(m)} = \mathbf{X}\hat{\beta}^{\text{pls}}(m)$. These linear coefficients can be recovered from the sequence of PLS transformations.
```