

Semi-Supervised Regression and System Identification

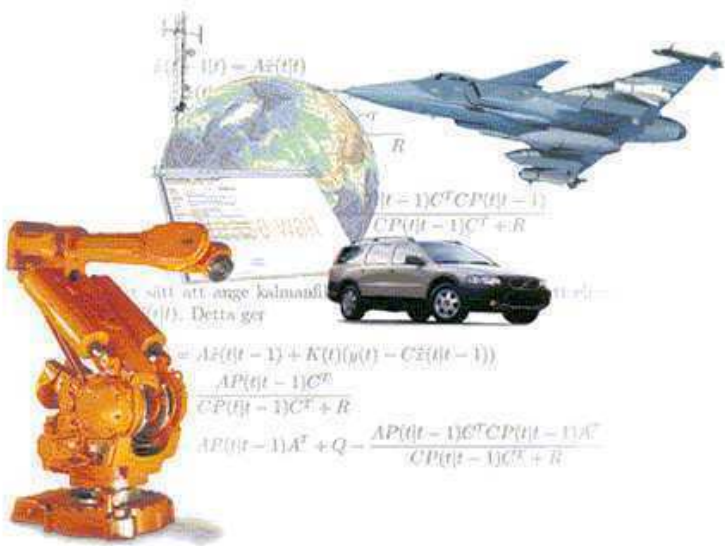
Lennart Ljung

Coauthor: Henrik Ohlsson

Division of Automatic Control

Linköping University

Sweden



Given a standard regression problem:

$$y(t) = f(\varphi(t)) + \text{noise}$$

f unknown, $y(t)$ and $\varphi(t)$ observed for $t = 1, \dots, N_L$. Find f !



Given a standard regression problem:

$$y(t) = f(\varphi(t)) + \text{noise}$$

f unknown, $y(t)$ and $\varphi(t)$ observed for $t = 1, \dots, N_L$. Find f !

Or rather, for any given φ^* find a good value of $f(\varphi^*)$ (“Model on Demand”, “Just in time model”)



Given a standard regression problem:

$$y(t) = f(\varphi(t)) + \text{noise}$$

f unknown, $y(t)$ and $\varphi(t)$ observed for $t = 1, \dots, N_L$. Find f !

Or rather, for any given φ^* find a good value of $f(\varphi^*)$ (“Model on Demand”, “Just in time model”)

Extra feature: We have several measurements of $\varphi(t)$, $t = N_L + 1, \dots, N_L + N_U$ without corresponding values of $y(t)$ (“unlabeled observations”)

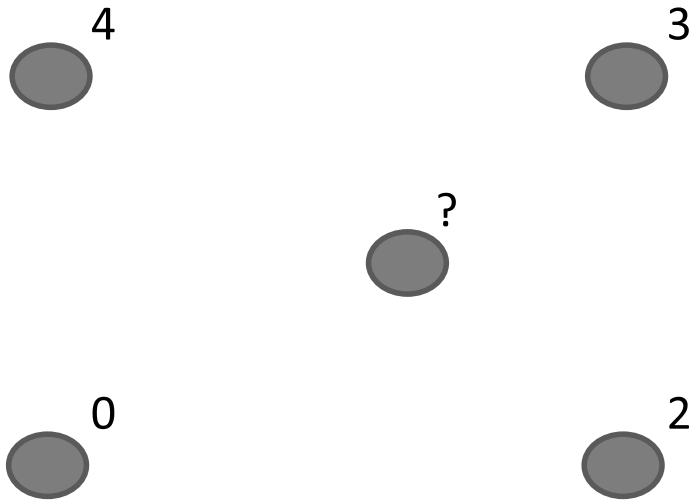




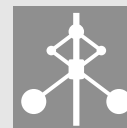
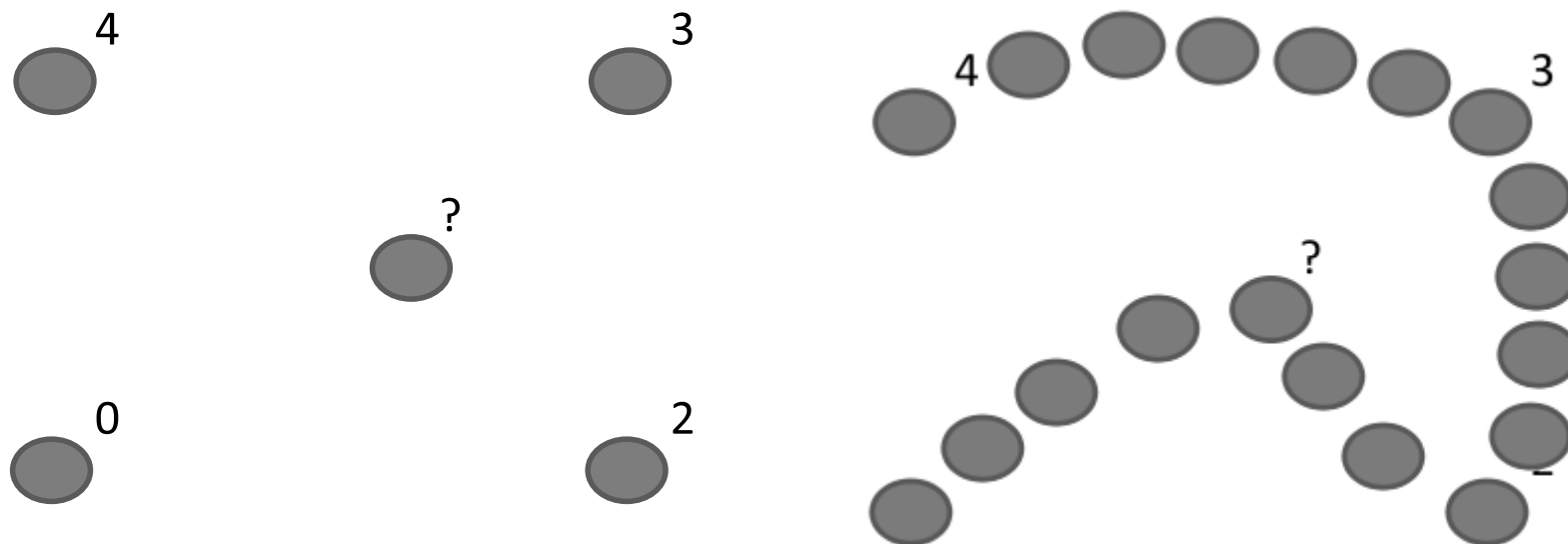
Yes, if the regressors live in a confined region, like a manifold:



Yes, if the regressors live in a confined region, like a manifold:



Yes, if the regressors live in a confined region, like a manifold:



- Supervised: All Regressors labeled $(y(t), \varphi(t))$ [Standard Regression problems]
- Unsupervised: No labels known. [Clustering, Classification]
- Semi-supervised: Some labels known $\{y(t), \varphi(t), t = 1, \dots, N_L\}$.
Some additional regressors known without labels
 $\{\varphi(t), t = N_L + 1, \dots, N_L + N_U\}$
- Estimation problem: still to “predict” $y^* = f(\varphi^*)$ for any given φ^*
 - “predict”:



WDMR: Weight Determination by Manifold Regression



WDMR: Weight Determination by Manifold Regression

(Manifold) Smoothness Assumption: $f(\varphi_1)$ and $f(\varphi_2)$ close if φ_1 and φ_2 are close (in a relevant metric).



WDMR: Weight Determination by Manifold Regression

(Manifold) Smoothness Assumption: $f(\varphi_1)$ and $f(\varphi_2)$ close if φ_1 and φ_2 are close (in a relevant metric).

Problem: associate $\varphi(i)$ with good values $\hat{f}_t = f(\varphi(t))$ for all regressors, both labeled and unlabeled.



WDMR: Weight Determination by Manifold Regression

(Manifold) Smoothness Assumption: $f(\varphi_1)$ and $f(\varphi_2)$ close if φ_1 and φ_2 are close (in a relevant metric).

Problem: associate $\varphi(i)$ with good values $\hat{f}_t = f(\varphi(t))$ for all regressors, both labeled and unlabeled.

Take care of two kinds of information:

- $f(\varphi(t)) \approx y(t)$ for the measured labels
- $f(\varphi(t)) \approx$ a weighted sum of $f(\varphi(j))$ for neighboring $\varphi(j) \approx \varphi(t)$ for all regressors



WDMR: Weight Determination by Manifold Regression

(Manifold) Smoothness Assumption: $f(\varphi_1)$ and $f(\varphi_2)$ close if φ_1 and φ_2 are close (in a relevant metric).

Problem: associate $\varphi(i)$ with good values $\hat{f}_t = f(\varphi(t))$ for all regressors, both labeled and unlabeled.

Take care of two kinds of information:

- $f(\varphi(t)) \approx y(t)$ for the measured labels
- $f(\varphi(t)) \approx$ a weighted sum of $f(\varphi(j))$ for neighboring $\varphi(j) \approx \varphi(t)$ for all regressors

Formalize the second information using a *kernel* $K(\cdot, \cdot)$:

$$\hat{f}_t \approx \sum_{t=1}^{N_L+N_U} K_{t,j} \hat{f}_j; \quad K_{t,j} = K(\varphi(t), \varphi(j))$$



Now, weigh together the two sources of information

$$\lambda \sum_{i=1}^{N_L+N_U} (\hat{f}_i - \sum_{j=1}^{N_L+N_U} K_{i,j} \hat{f}_j)^2 + (1 - \lambda) \sum_{t=1}^{N_L} (y(t) - \hat{f}_t)^2 \quad (*)$$

$$K_{i,j} = K(\varphi(i), \varphi(j))$$

Pick a (“regularization parameter”) λ that balances the fit to measured labels and the smoothness prior. Minimize w.r.t. $\hat{f}_t, t = 1, \dots, N_L + N_U$.



Now, weigh together the two sources of information

$$\lambda \sum_{i=1}^{N_1+N_u} (\hat{f}_i - \sum_{j=1}^{N_L+N_U} K_{i,j} \hat{f}_j)^2 + (1 - \lambda) \sum_{t=1}^{N_L} (y(t) - \hat{f}_t)^2 \quad (*)$$

$$K_{i,j} = K(\varphi(i), \varphi(j))$$

Pick a (“regularization parameter”) λ that balances the fit to measured labels and the smoothness prior. Minimize w.r.t. $\hat{f}_t, t = 1, \dots, N_L + N_U$.

That gives the estimated function value $\hat{f}(\varphi)$ for any regressor φ you include among the unlabeled regressors.



Now, weigh together the two sources of information

$$\lambda \sum_{i=1}^{N_1+N_u} (\hat{f}_i - \sum_{j=1}^{N_L+N_U} K_{i,j} \hat{f}_j)^2 + (1 - \lambda) \sum_{t=1}^{N_L} (y(t) - \hat{f}_t)^2 \quad (*)$$

$$K_{i,j} = K(\varphi(i), \varphi(j))$$

Pick a (“regularization parameter”) λ that balances the fit to measured labels and the smoothness prior. Minimize w.r.t. $\hat{f}_t, t = 1, \dots, N_L + N_U$.

That gives the estimated function value $\hat{f}(\varphi)$ for any regressor φ you include among the unlabeled regressors.

Note that $(*)$ is quadratic in \hat{f}_t , so the solution is easy to obtain.



Many possibilities: K -Nearest Neighbors, Gaussian Kernels



Many possibilities: K -Nearest Neighbors, Gaussian Kernels

Choice that can adapt the metric to manifolds and other high-density regions:
Local Linear Embedding (LLE):



Many possibilities: K -Nearest Neighbors, Gaussian Kernels

Choice that can adapt the metric to manifolds and other high-density regions:
Local Linear Embedding (LLE):

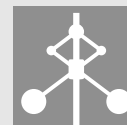
Find the Kernel $K_{i,j} = K(\varphi(i), \varphi(j))$ by minimizing (wrt $K_{i,j}$)

$$\varepsilon(K) = \sum_{i=1}^N \left\| \varphi(i) - \sum_{j=1}^N K_{i,j} \varphi(j) \right\|^2 \quad (3a)$$

under the constraints

$$\begin{cases} \sum_{j=1}^N K_{i,j} = 1, & K_{i,i} = 0 \\ K_{i,j} = 0 \text{ if } \|\varphi(i) - \varphi(j)\| > C_i(R) \text{ or if } i = j. \end{cases} \quad (3b)$$

Here, $C_i(R)$ is chosen so that only R weights $K_{i,j}$ become nonzero for every i . R is a design variable.



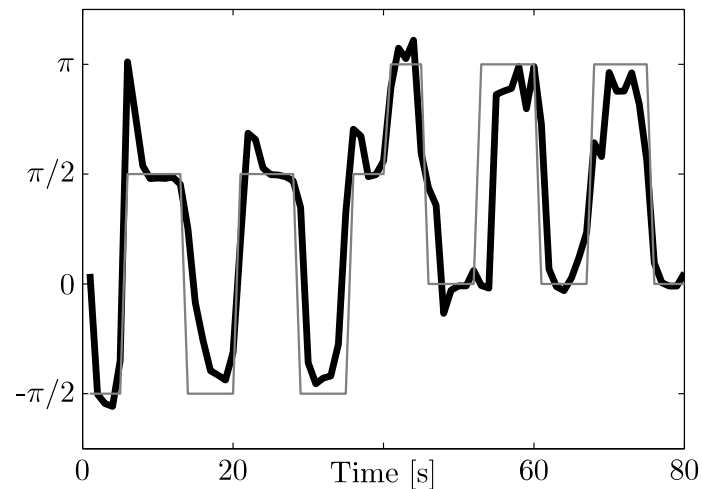


The patient in the magnet camera is moving his eye focus left - right - up - down. 128 voxels in the visual cortex are monitored by fMRI, giving a vector $\varphi(t) \in R^{128}$ sampled every two seconds. The output $y(t)$ is the viewing angle $0, \pi, \pi/2, -\pi/2$.



120 (labeled) samples were collected. 80 of those were treated as “labeled” ($N_L = 80$) and the remaining 40 were treated as “unlabeled” ($N_U = 40$).

Below we show the predicted y -values ($[-\pi/2 \ \pi]$), (thick line) for these unlabeled measurements together with the corresponding true angles (thin line).



Equation: (Biological interpretation)

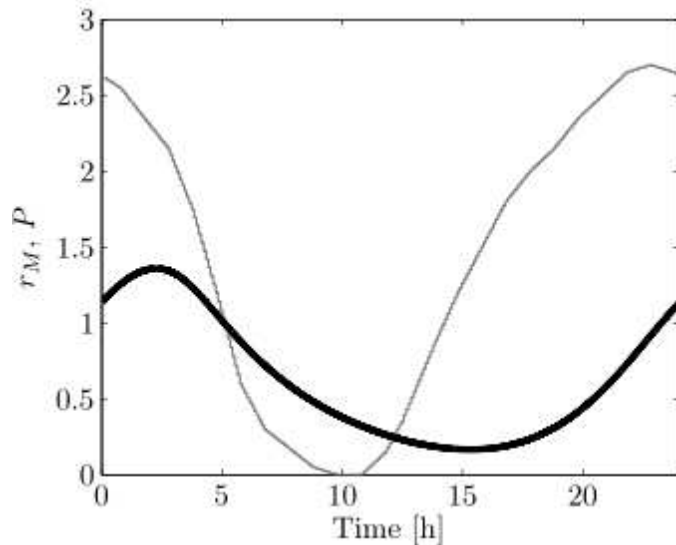
$$\frac{dM(t)}{dt} = \frac{r_M(t)}{1 + P(t)^2} - 0.21M(t),$$
$$\frac{dP(t)}{dt} = M(t - 4)^3 - 0.21P(t),$$

Input $r_M(t)$ (periodic, cheap), Output $P(t)$ (expensive)

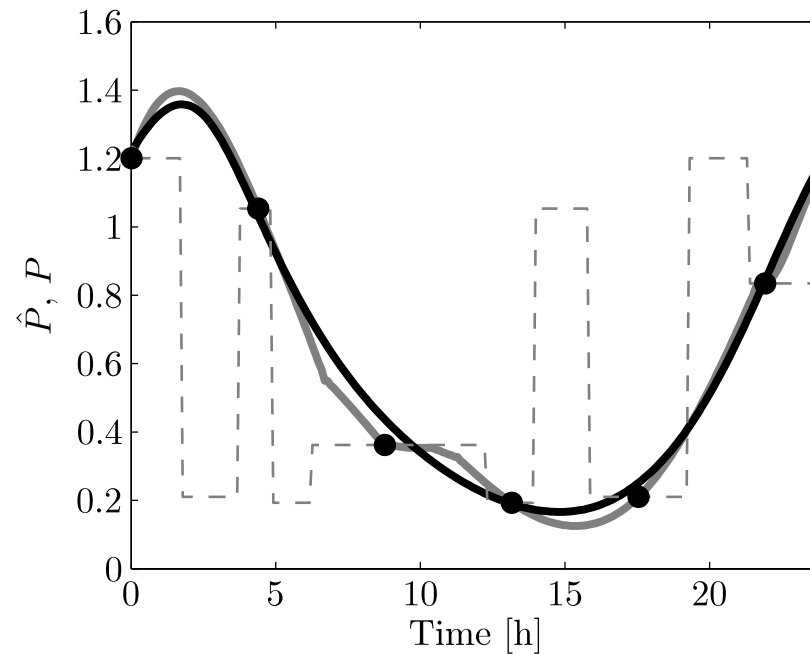
Predict P from r_M . Use $[r_M(t) \ r_M(t - 4)]^T$ as regression vector



Measured Data



Estimated output (black line)
true output (grey line)
measured outputs (6 dots)
[Dashed: Near.t Neighb. estimates]



Note that only 6 P-values are measured.
($t=0, 4, 9, 14, 17, 22$)



$$x_1(t+1) = \left(\frac{x_1(t)}{1+x_1^2(t)} + 1 \right) \sin(x_2(t))$$

$$x_2(t+1) = x_2(t) \cos(x_2(t)) + x_1(t) \exp\left(-\frac{x_1^2(t) + x_2^2(t)}{8}\right) + \frac{u^3(t)}{1+u^2(t) + 0.5 \cos(x_1(t) + x_2(t))}$$

$$y(t) = \frac{x_1(t)}{1+0.5 \sin(x_2(t))} + \frac{x_2(t)}{1+0.5 \sin(x_1(t))} + e(t)$$

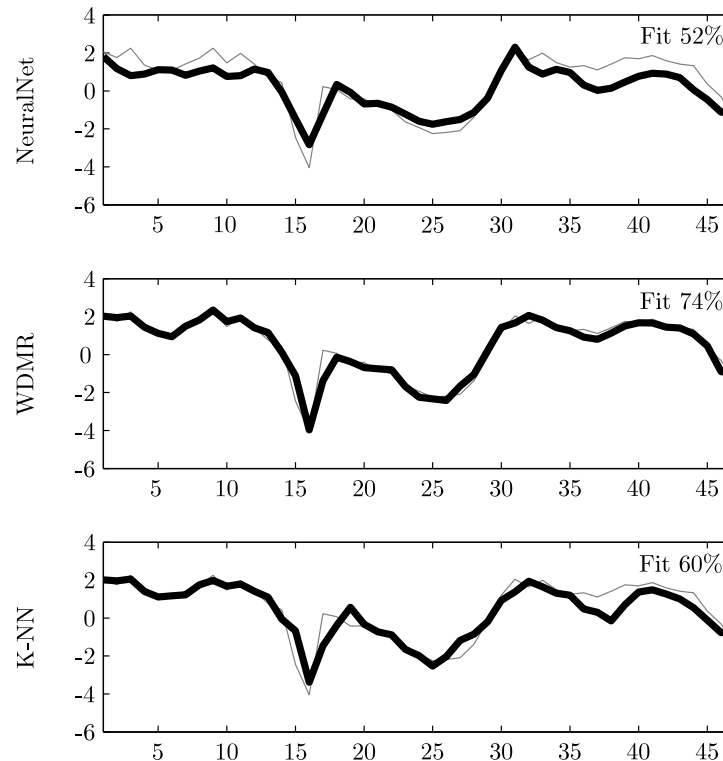
u : **RBS** for estimation data; **sinusoid** for validation data

Regression vector.

$$\varphi(t) = [y(t-1)y(t-2), y(t-3), u(t-1), u(t-2), u(t-3)]^T \text{ [NLARX]}$$



One-step ahead prediction on validation data



Top: Standard Neural Network (18 hidden units — best) **52% fit**

Middle: WDMR ($\lambda = 0.5$, LLE kernel $R=5$) **74% fit**

Bottom: K -nearest neighbor ($K = 15$ — best) **60% fit**



- Ideas from “machine learning” have relevance for system identification
- A method WDMR was suggested for non-linear regression
 - Local, non-parametric flavor
 - Links to LLE
- It shows promising results for several examples of different characters
- More to understand regarding the potential for system identification!

