CS373 Data Mining and Machine Learning

Lecture 7

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(originally prepared by Tommi Jaakkola, MIT CSAIL)

Today's topics

- Preface: regression
  - linear regression, kernel regression
- Feature selection
  - information ranking, regularization, subset selection

Linear regression

- We seek to learn a mapping from inputs to continuous valued outputs (e.g., price, temperature)
- The mapping is assumed to be linear in the feature space so that the predicted output is given by

$$\hat{y}(\underline{x}) = \underline{\theta} \cdot \underline{\phi}(\underline{x})$$

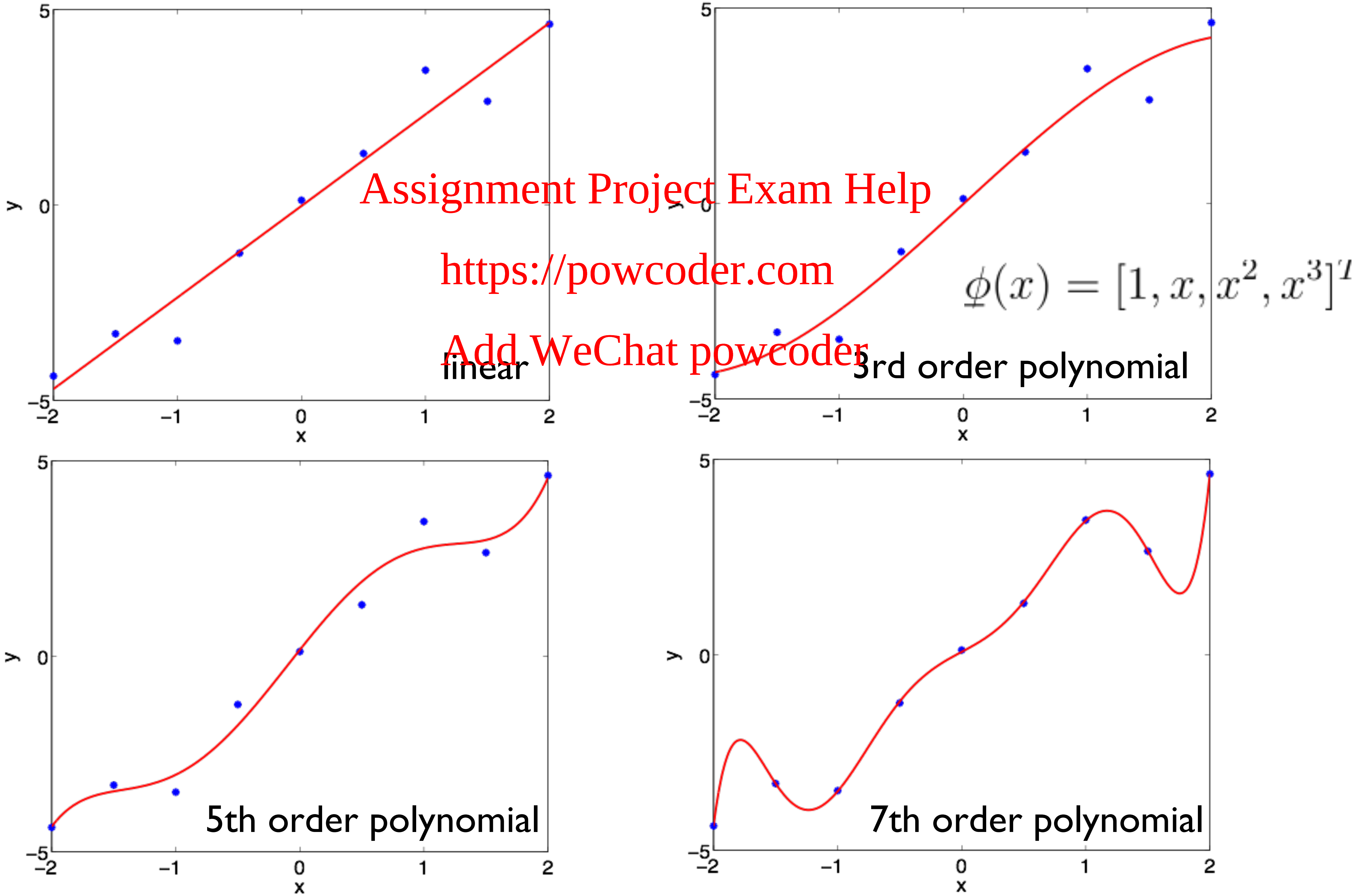
- Assuming that the noise in the observed outputs is additive zero mean Gaussian we can obtain the parameters from training samples by minimizing

$$J(\underline{\theta}) = \underbrace{\frac{1}{2}\sum_{t=1}^{n}}_{\text{sum over the training examples}} \underbrace{\left(y_t - \underline{\theta} \cdot \underline{\phi}(\underline{x}_t)\right)^2}_{\text{squared prediction loss on the example}} + \underbrace{\frac{\lambda}{2}\|\underline{\theta}\|^2}_{\text{regularization term}}$$

- The regularization term guarantees that any unused parameter dimensions are set to zero

Linear regression

- We can easily obtain non-linear regression functions by considering different feature mappings



Linear regression solution

$$J(\underline{\theta}) = \frac{1}{2}\sum_{t=1}^{n}\left(y_t - \underline{\theta}\cdot\underline{\phi}(\underline{x}_t)\right)^2 + \frac{\lambda}{2}\|\underline{\theta}\|^2$$

$$\frac{d}{d\underline{\theta}}J(\underline{\theta}) = \sum_{t=1}^{n} - \overbrace{\left(y_t - \underline{\theta}\cdot\underline{\phi}(\underline{x}_t)\right)}^{\alpha_t}\underline{\phi}(\underline{x}_t) + \lambda\underline{\theta} = 0$$

$$\Rightarrow \underline{\theta}(\alpha) = \frac{1}{\lambda}\sum_{t=1}^{n}\alpha_t\underline{\phi}(\underline{x}_t)$$

- The unique solution lies in the span of the feature vectors (this is due to the regularization term)

Dual linear regression

- The dual parameters are obtained as the solution to a linear equation

$$\alpha_t = y_t - \underline{\theta}(\alpha) \cdot \underline{\phi}(\underline{x}_t)$$
$$= y_t - \frac{1}{\lambda} \sum_{i=1}^{n} \alpha_i \underbrace{[\underline{\phi}(\underline{x}_i) \cdot \underline{\phi}(\underline{x}_t)]}_{\text{kernel } K(\underline{x}_i, \underline{x}_t)}$$

$$\Rightarrow \underbrace{\alpha^*}_{n \times 1} = (I + \frac{1}{\lambda} \underbrace{K}_{n \times n \text{ Gram matrix}})^{-1} \underbrace{y}_{n \times 1}$$

- Predicted output for a new input is given by

$$\hat{y}(\underline{x}) = \underline{\theta}(\alpha^*) \cdot \underline{\phi}(\underline{x}) = \frac{1}{\lambda} \sum_{i=1}^{n} \alpha_i^* \underbrace{[\underline{\phi}(\underline{x}_i) \cdot \underline{\phi}(\underline{x})]}_{\text{kernel } K(\underline{x}_i, \underline{x})}$$

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Coordinate selection

- Linear models

classification

$$y = \text{sign}\big(\,\underline{\theta} \cdot \underline{\phi}(\underline{x})\,\big) \in \{-1, 1\}$$

regression

$$y = \underline{\theta} \cdot \underline{\phi}(\underline{x}) \in \mathcal{R}$$

etc.

feature coordinate

$$\underline{\phi}(\underline{x}) = \begin{bmatrix} \phi_1(\underline{x}) \\ \cdots \\ \phi_d(\underline{x}) \end{bmatrix}$$

- We seek to identify a few feature coordinates that the class label or regression output primarily depends on
- This is often advantageous in order to improve generalization (as feature selection exerts additional complexity control) or to gain interpretability

Simple coordinate selection

- There are a number of different approaches to coordinate selection
- Information analysis
  - rank individual features according to their mutual information with the class label
  - limited to discrete variables
- 1-norm regularization
  - replaces the two-norm regularizer with 1-norm that encourages some of the coordinates to be set exactly to zero
- Iterative subset selection
  - iteratively add (or prune) coordinates based on their impact on the (training) error

Information analysis

- Suppose the feature vector is just the input vector x whose coordinates take values in {1,...,k}
- Given a training set of size n, we can evaluate an empirical estimate of the mutual information between the coordinate values and the binary label

$$\hat{I}(Y, X_i) = \sum_{y \in \{-1,1\}} \sum_{x_i=1}^{k} \hat{P}(y, x_i) \log \frac{\hat{P}(y, x_i)}{\hat{P}(y)\hat{P}(x_i)}$$

$$\hat{P}(y, x_i) = \frac{1}{n} \sum_{t=1}^{n} \delta(y, y_t)\underline{\delta(x_i, x_{ti})}$$

$$\begin{cases} 1, & \text{if } x_i = x_{it} \\ 0, & \text{otherwise} \end{cases}$$

empirical estimates

$$\hat{P}(y) = \frac{1}{n} \sum_{t=1}^{n} \delta(y, y_t)$$

$$\hat{P}(x_i) = \frac{1}{n} \sum_{t=1}^{n} \delta(x_i, x_{it})$$

Information analysis

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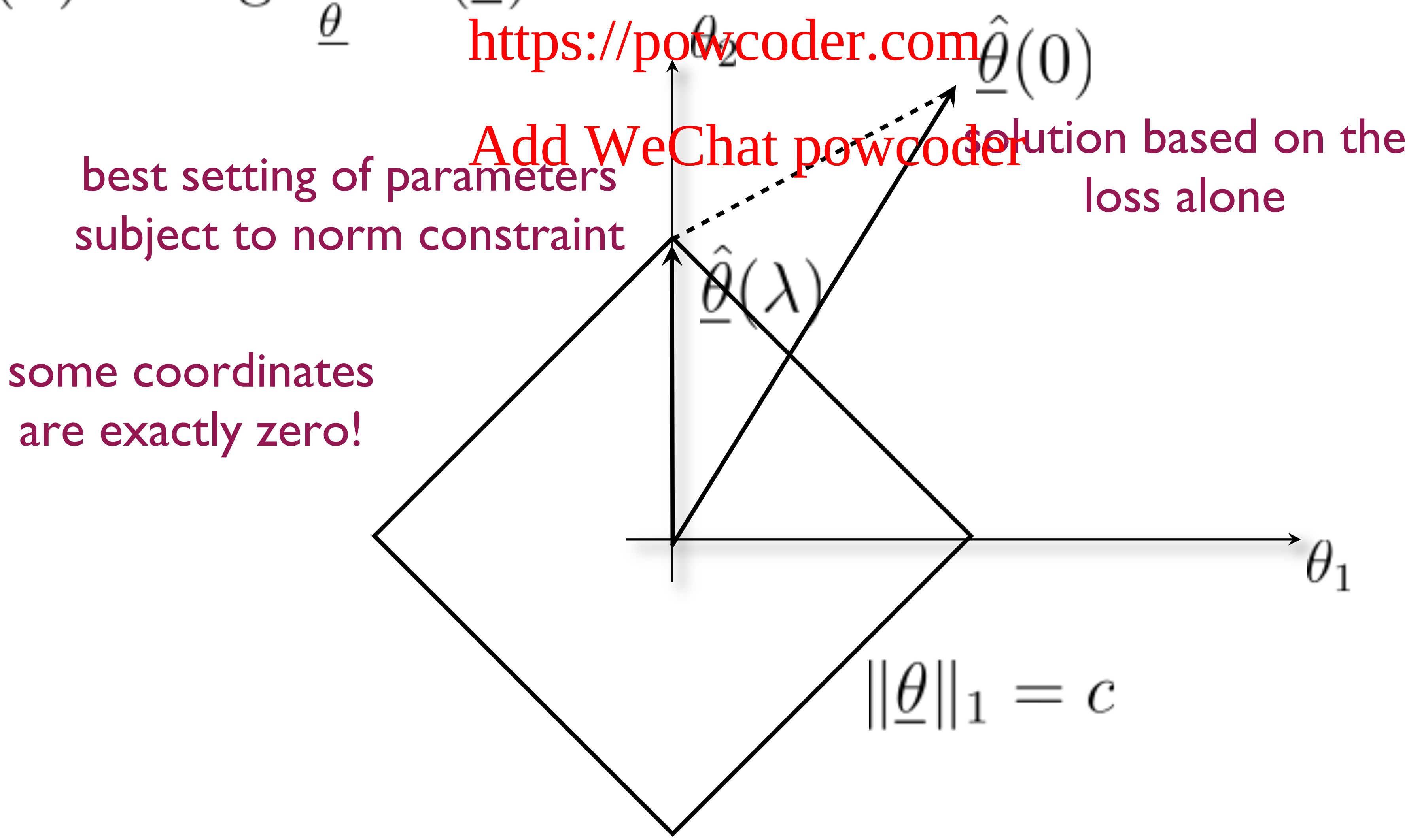
  - provides a ranking of the features to include
  - weights redundant features equally (would include neither or both)
  - not tied to the linear classifier (may select features that the linear classifier cannot use, or omit combinations of features particularly useful in a linear classifier)

Regularization approach (Lasso)

- By using a 1-norm regularizer we will cause some of parameters to be set exactly to zero

$$J(\underline{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(y_t - \underline{\theta}\cdot\phi(\underline{x}_i)\right)^2 + \lambda\|\underline{\theta}\|_1$$

$$\hat{\underline{\theta}}(\lambda) = \underset{\underline{\theta}}{\operatorname{argmin}}\, J(\underline{\theta})$$



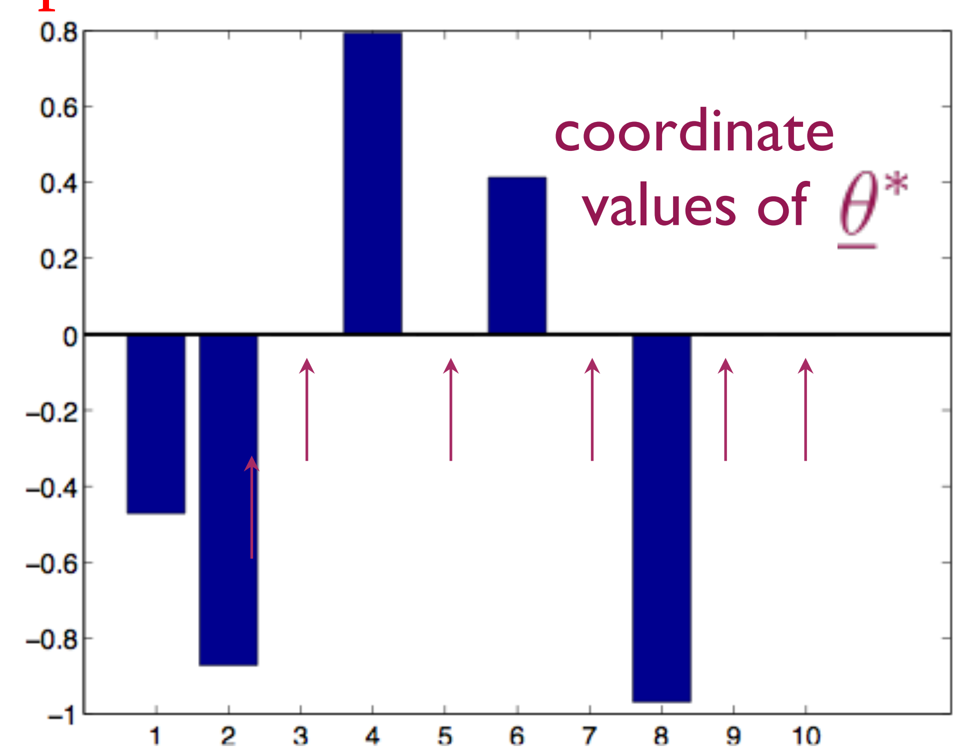
Regularization example

- n=100 samples, d=10, training outputs generated from

$$y_t \sim N\left(\underline{\theta}^* \cdot \underline{x}_t,\, \sigma^2\right),\ t = 1, \ldots, n$$

- If we increase the regularization penalty, we get fewer non-zero parameters in the solution to

$$J(\underline{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(y_t - \underline{\theta}\cdot\phi(\underline{x}_i)\right)^2 + \lambda\|\underline{\theta}\|_1$$



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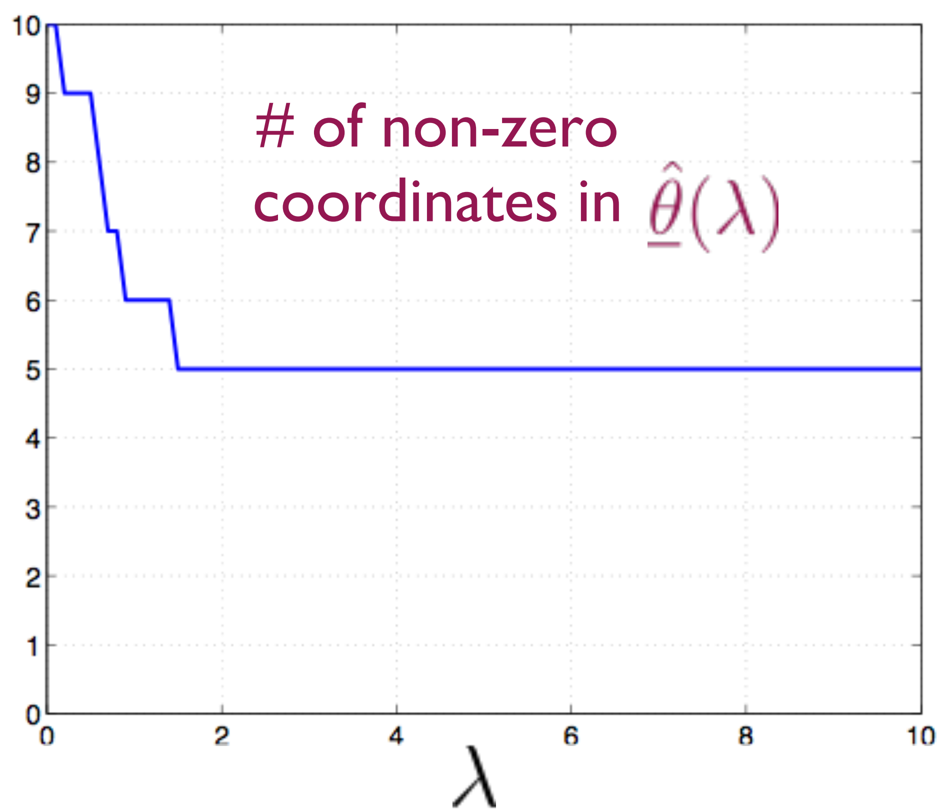
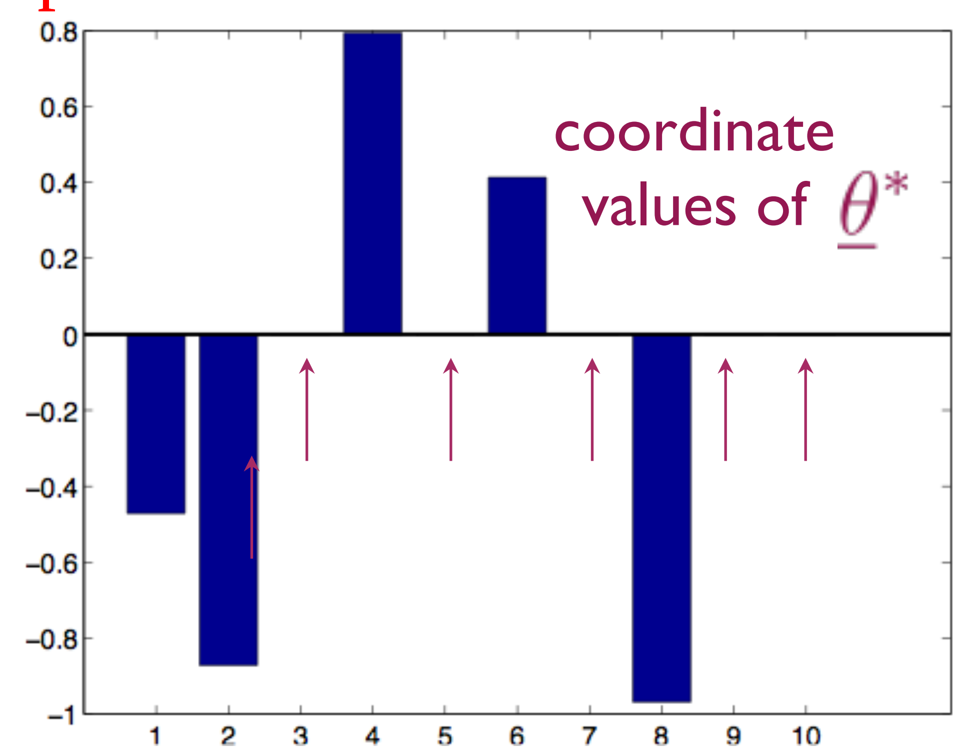




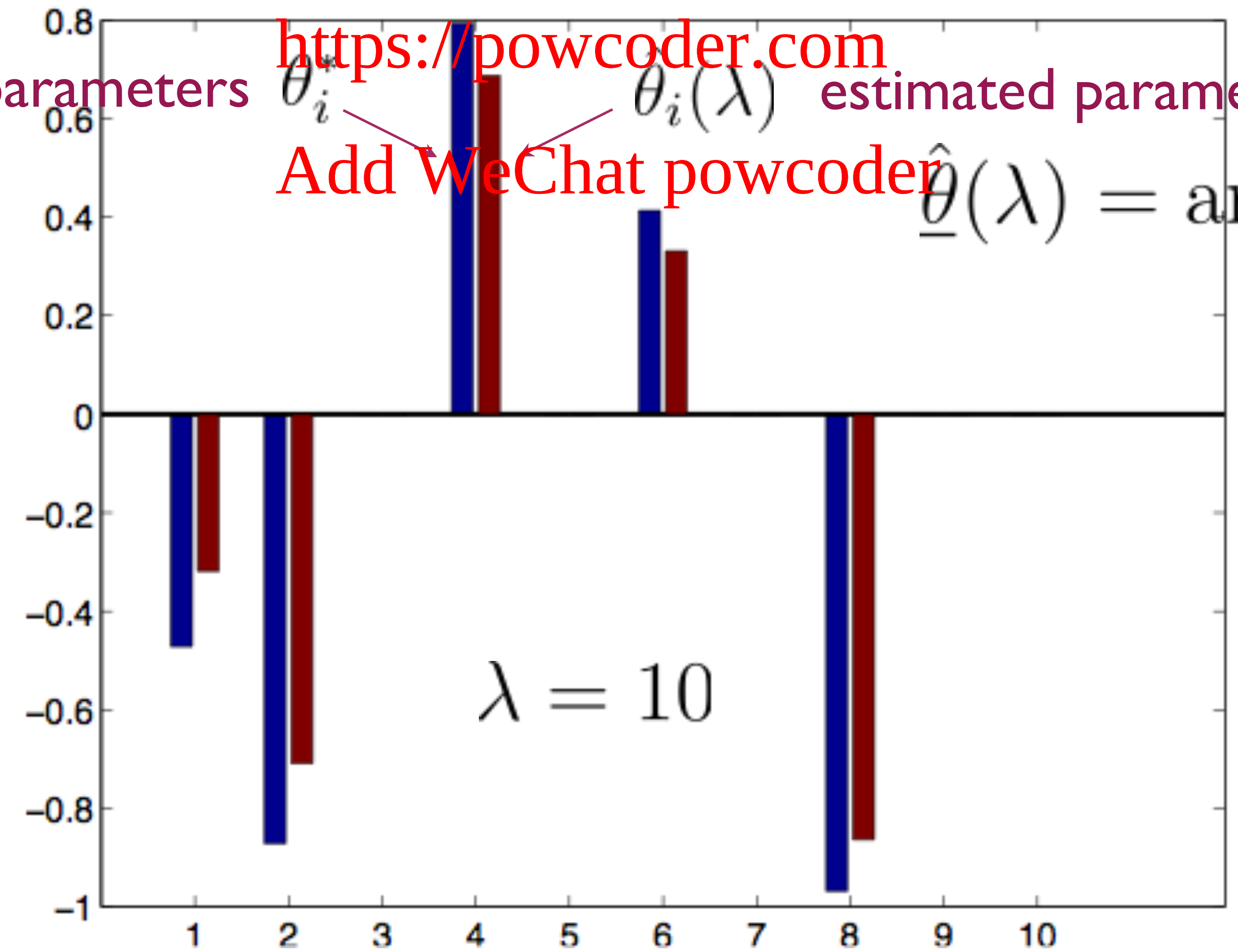
Regularization example

- The 1-norm penalty term controls the number of non-zero coordinates but also reduces the magnitude of the coordinates

$$J(\underline{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(y_t - \underline{\theta}\cdot\underline{\phi}(\underline{x}_i)\right)^2 + \lambda\|\underline{\theta}\|_1$$

true parameters θ_i^* $\hat{\theta}_i(\lambda)$ estimated parameters

$$\underline{\hat{\theta}}(\lambda) = \underset{\underline{\theta}}{\mathrm{argmin}}\, J(\underline{\theta})$$



Subset selection

- A greedy algorithm for finding a good subset of feature coordinates (feature functions) to rely on

$$\phi_1(\underline{x}), \ldots, \phi_d(\underline{x}) \qquad \phi_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j \in S}$$

for each subset S, $|S| = k$, evaluate

$$J(S) = \min_{\underline{\theta}_S} \frac{1}{2} \sum_{t=1}^{n} \left(y_t - \underline{\theta}_S \cdot \underline{\phi}_S(\underline{x}_t)\right)^2$$

each feature subset is assessed on the basis of the resulting training error

$$\hat{S} = \underset{S}{\operatorname{argmin}}\, J(S)$$

find the best subset

- k is used for (statistical) complexity control
- computationally hard (exponential in k)

Greedy subset selection

- A greedy algorithm for finding a good subset of feature coordinates (feature functions) to rely on

$$\phi_1(\underline{x}), \ldots, \phi_d(\underline{x}) \qquad \phi_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j \in S}$$

$$S = \emptyset$$

for each $j \notin S$ evaluate

try each new coordinate

$$J(S \cup j) = \min_{\underline{\theta}_{S \cup j}} \frac{1}{2} \sum_{t=1}^{n} \left(y_t - \underline{\theta}_{S \cup j} \cdot \underline{\phi}_{S \cup j}(\underline{x}_t) \right)^2$$

re-estimate all the parameters in the context of the new coordinate

$$\hat{j} = \operatorname*{argmin}_{j \notin S} J(S \cup j)$$

find the best coordinate to include

$$S \leftarrow S \cup \{\hat{j}\}$$

  - each new feature is assessed in the context of those already included
  - the method is not guaranteed to find the optimal subset

Forward-fitting

- We can also choose feature coordinates without re-estimating the parameters associated with already included coordinates

$$\phi_1(\underline{x}), \ldots, \phi_d(\underline{x}) \qquad \underline{\phi}_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j \in S}$$

$$S = \emptyset, \quad \underline{\hat{\theta}}_\emptyset = 0$$

for each j evaluate

fixed at this stage

$$J(\underline{\hat{\theta}}_S, j) = \min_{\theta_j} \frac{1}{2} \sum_{t=1}^{n} \left(y_t - \underline{\hat{\theta}}_S \cdot \underline{\phi}_S(\underline{x}_t) - \underline{\theta_j \phi_j(\underline{x}_t)} \right)^2$$

re-estimate only the parameter associated with the new coordinate

$$\hat{j} = \underset{j}{\operatorname{argmin}}\, J(\underline{\hat{\theta}}_S, j)$$

select the best new feature

$$\underline{\hat{\theta}}_{S \cup j} = \{\underline{\hat{\theta}}_S, \hat{\theta}_{\hat{j}}\}, \quad S \leftarrow S \cup \{\hat{j}\},$$

- same feature may be included more than once

Myopic forward fitting

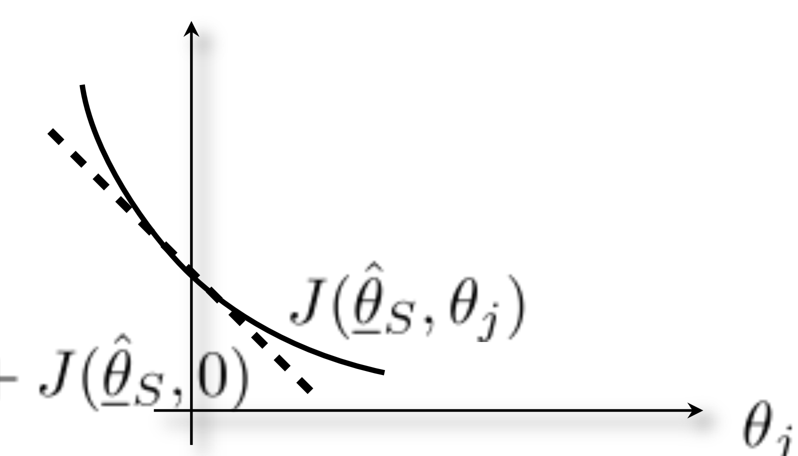
- We can also identify new features in a more limited way by focusing on how much "potential" each feature has for reducing the training error

$$\phi_1(\underline{x}), \ldots, \phi_d(\underline{x}) \qquad \underline{\phi}_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j\in S}$$

$$J(\underline{\hat{\theta}}_S, \theta_j) = \frac{1}{2}\sum_{t=1}^{n}\left(y_t - \underline{\hat{\theta}}_S \cdot \underline{\phi}_S(\underline{x}_t) - \theta_j \phi_j(\underline{x}_t)\right)^2$$

$$DJ(\underline{\hat{\theta}}_S, j) = \frac{\partial J(\underline{\hat{\theta}}_S, \theta_j)}{\partial \theta_j}\Big|_{\theta_j=0} = -\sum_{t=1}^{n}\left(y_t - \underline{\hat{\theta}}_S \cdot \underline{\phi}_S(\underline{x}_t)\right)\phi_j(\underline{x}_t)$$

|derivative| is large if the corresponding feature would have a large effect on the error



Myopic forward fitting

- We can identify new features with minimal fitting

$$\phi_1(\underline{x}), \ldots, \phi_d(\underline{x}) \qquad \underline{\phi}_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j \in S}$$

$$S = \emptyset, \quad \underline{\hat{\theta}}_\emptyset = 0$$

for each j evaluate

fixed at this stage

$$DJ(\underline{\hat{\theta}}_S, j) = \frac{\partial J(\underline{\hat{\theta}}_S, \theta_j)}{\partial \theta_j}\bigg|_{\theta_j = 0}$$

the criterion does not involve any parameter fitting

$$\hat{j} = \operatorname*{argmax}_j |DJ(\underline{\hat{\theta}}_S, j)|$$

selection of best coordinate

$$\hat{\theta}_{\hat{j}} = \operatorname*{argmin}_{\theta_{\hat{j}}} J(\underline{\hat{\theta}}_S, \theta_{\hat{j}})$$

estimate only the parameter associated with the selected feature

$$\underline{\hat{\theta}}_{S \cup \hat{j}} = \{\underline{\hat{\theta}}_S, \hat{\theta}_{\hat{j}}\}, \quad S \leftarrow S \cup \{\hat{j}\},$$

Forward-fitting example

- 1 dimensional polynomial regression

$$\underline{\phi}(x) = [1, x, x^2, x^3, x^4]^T \qquad \underline{\phi}_S(\underline{x}) = \{\phi_j(\underline{x})\}_{j\in S}$$

$$J(\hat{\underline{\theta}}_S, \theta_j) = \frac{1}{2}\sum_{t=1}^{n}\left(y_t - \hat{\underline{\theta}}_S \cdot \underline{\phi}_S(\underline{x}_t) - \theta_j\phi_j(\underline{x}_t)\right)^2$$

iter	deg	$\hat{\theta}_{\hat{j}}$	$J(\hat{\underline{\theta}})$
1	0	$+1.089$	0.874
2	1	-0.553	0.163
3	2	-0.288	0.085
4	1	-0.101	0.062
5	0	-0.033	0.051
6	3	$+0.053$	0.049
7	1	-0.043	0.045
8	3	$+0.088$	0.041
9	1	-0.035	0.039
10	3	$+0.072$	0.036

forward-fitting

iter	deg	$\hat{\theta}_{\hat{j}}$	$J(\hat{\underline{\theta}})$
1	0	$+1.089$	0.874
2	1	-0.553	0.163
3	0	-0.085	0.091
4	1	-0.056	0.084
5	2	-0.127	0.069
6	0	$+0.021$	0.065
7	1	-0.031	0.063
8	2	-0.078	0.057
9	0	$+0.013$	0.055
10	1	-0.018	0.054

myopic forward-fitting

Forward-fitting example

- 1 dimensional polynomial regression

$$\phi(x) = [1, x, x^2, x^3, x^4]^T$$