Learning in Big Data Analytics
Lecture 2

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Supervised Learning

Supervised Learning

- There is a functional relationship

$$f^* : \mathbb{R}^d \to V$$

we would like to understand, or *learn*.

  - *Regression*: $V = \mathbb{R}$
  - *Classification*: $V = \{1, ..., k\}$
- To learn it, we are given *m data points*

$$(x_i, f^*(x_i) = y_i)_{i=1,...,m}$$

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  that reflect this functional relationship.

Final goal: Predict $f^*(x)$ well on unknown data points x.

Supervised versus Unsupervised Learning

- *Unsupervised Learning:*
  - Given unlabeled data

$$(x_i)_{i=1,\dots,m}$$

  - *Goal:* Infer subgroups of data points
  - *Alternative Problem Formulation:* Learn the probability distribution

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EXAMPLE

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Example

Supervised Learning: Training

- The idea is to set up a *training procedure* (an algorithm) that *learns* f^* from the training data.
- Learning f^* means to *approximate* it by $f : \mathbb{R}^d \to V$ sufficiently well, where $f \in \mathcal{M}$ for a certain class of functions $\mathcal{M}$.
- In most cases, $f \in \mathcal{M}$ are parameterized by parameters $\mathbf{w}$. This means that we have to pick an appropriate choice of parameters $\mathbf{w}$ for learning f^*.

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SUPERVISED LEARNING

- We need to determine a *cost (or loss) function* C where $C(f, f^*)$ measures how well $f \in \mathcal{M}$ approximates f^*.
- *Optimization*: Pick $f \in \mathcal{M}$ (by picking the right set of parameters) that yields small (possibly minimal) cost $C(f, f^*)$
- *Generalization*: Optimization procedure should address that f is to approximate f^* well on *unknown data points*.

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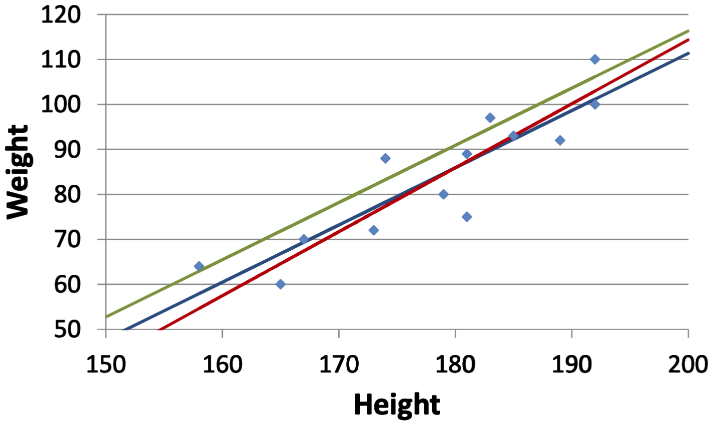
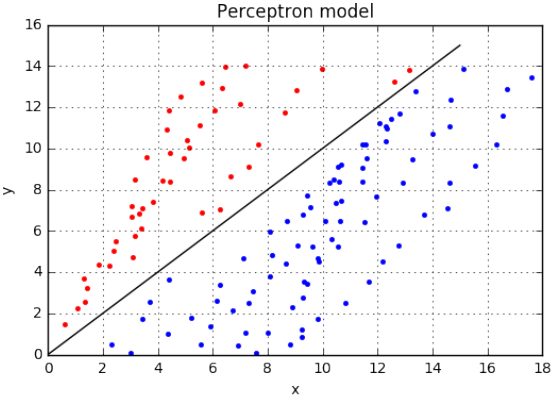
Linear Regression

Example: $f : \mathbb{R} \to \mathbb{R}$



Perceptron

Example: $f : \mathbb{R}^2 \to \{0, 1\}$



$$
\begin{array}{lccc}
f & \mathbb{R}^2 & \longrightarrow & \{0 = \text{blue}, 1 = \text{red}\} \\
 & (x_1, x_2) & \mapsto & \begin{cases} 1 & x_2 - x_1 > 0 \\ 0 & x_2 - x_1 \leq 0 \end{cases}
\end{array}
\tag{1}
$$

We need to specify:

- How to set up the data being used for training
- A model class $\mathcal{M}$, for example linear functions
- A cost function $C(f, f^*)$ that evaluates the goodness of $f \in \mathcal{M}$
- An optimization procedure that picks f such that $C(f, f^*)$ is minimal, or very small
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Supervised Learning

Notation

- The dataset is given by a *design matrix* $\mathbf{X} \in \mathbb{R}^{m \times d}$ where m is the number of data points and d is the number of *features*
- Each data point x_i (a row in $\mathbf{X}$) is assigned to a *label* y_i that reflects the true functional relationship $y_i = f^*(x_i)$, where further $\mathbf{y} = (y_1, ..., y_m) \in V^m$ is the *label vector*.

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Generalization

Enabling Generalization: Data

Training, Test and Validation

- Split $(\mathbf{X}, \mathbf{y})$ into
  - training data $(\mathbf{X}^{(\text{train})}, \mathbf{y}^{(\text{train})})$
  - validation data $(\mathbf{X}^{(\text{val})}, \mathbf{y}^{(\text{val})})$
  - test data $(\mathbf{X}^{(\text{test})}, \mathbf{y}^{(\text{test})})$
- While *training data* is to pick the optimal set of parameters (which specify elements from $\mathcal{M}$), using training and *validation data* in combination is for picking *hyperparameters*
- Hyperparameters can refer to choosing subsets of $\mathcal{M}$. For example, depth of a neural network, and widths of hidden layers. They may also refer to specifications of cost function or optimization procedure.
- $(\mathbf{X}^{(\text{test})}, \mathbf{y}^{(\text{test})})$ are never touched during training.
- The final goal is to minimize the cost on the test data.

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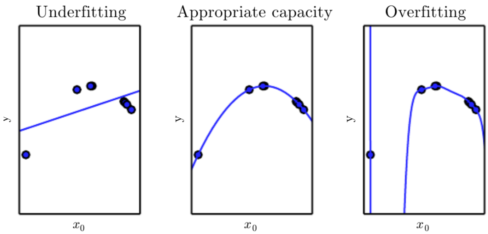
Enabling Generalization: Model

Capacity, Under- and Overfitting



Left: Linear functions underfit
Center: Polynomials of degree 2 neither under- nor overfit
Right: Polynomials of degree 9 overfit

- Choose a class of models that has the right *capacity*
- Capacity too large: *overfitting*
- Capacity too small: *underfitting*

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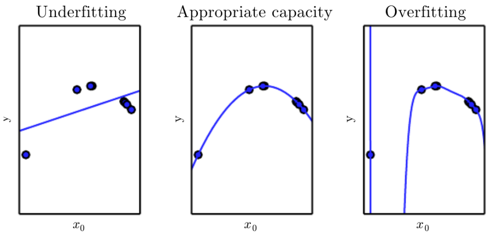

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Enabling Generalization: Cost Function

Regularization

Let $C(f, f^*)$ be the cost function. Let $\mathbf{w} = (w_1, ..., w_k)$ be the parameters specifying elements of $f_{\mathbf{w}} \in \mathcal{M}$.

- Usually, C refers to only known data points. That is, C evaluates as

$$C(f, f^*) = \sum_i C(f(x_i), y_i = f^*(x_i)) \quad (2)$$

where x_i runs over all training data points.

- Add a *regularization term* to cost function, and choose $f_{\mathbf{w}}$ that yields minimal

$$C(f_{\mathbf{w}}, f^*) + \lambda\Omega(\mathbf{w}) \quad (3)$$

- λ is a hyperparameter

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- Prominent examples:
  - *L_1 norm*: $\Omega(\mathbf{w}) := \sum_i |w_i|$
  - *L_2 norm*: $\Omega(\mathbf{w}) := \sum_i w_i^2$
- Rationale: Penalize too many non-zero weights
- Virtually less complex model, hence virtually less capacity
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Enabling Generalization: Optimization

Early Stopping, Dropout

Optimization can be an iterative procedure.

- *Early stopping*: Stop the optimization procedure before cost function reaches an optimum on the training data.
- *Dropout*: Randomly fix parameters to zero, and optimize remaining parameters.

Prominent Supervised Learning Model Examples

Linear Regression

- Design matrix $\mathbf{X} \in \mathbb{R}^{m \times d}$, label vector $\mathbf{y} \in \mathbb{R}^m$
- Model class: Let $\mathbf{w} \in \mathbb{R}^d$

$$f_{\mathbf{w}} = f(\mathbf{x}; \mathbf{w}) : \begin{array}{ccc} \mathbb{R}^d & \longrightarrow & \mathbb{R} \\ \mathbf{x} & \mapsto & \mathbf{w}^T\mathbf{x} \end{array} \tag{4}$$

- *Remark*: Note that the case $\mathbf{w}^T\mathbf{x} + b$ can be treated as a special case to be included in $\mathcal{M}$, by augmenting vectors $\mathbf{x}_i$ by an entry 1 (think about this...)
- Cost function (recall $y_i = f^*(\mathbf{x}_i)$)

$$C(f, f^*) := \frac{1}{m}||(f(\mathbf{x}_1), ..., f(\mathbf{x}_m)) - \mathbf{y}||_2^2 = \frac{1}{m}\sum_{i=1}^{m}(f(\mathbf{x}_i) - \mathbf{y}_i)^2 \tag{5}$$

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LINEAR REGRESSION

Optimization

- Solve for

$$\nabla_{\mathbf{w}} C(f_{\mathbf{w}}, f^*) = 0 \tag{6}$$

  to achieve a minimum. This yields the *normal equations*

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \tag{7}$$

- *Global optimum* if $\mathbf{X}^T\mathbf{X}$ is invertible
- Do this on *training data* (so $\mathbf{X} = \mathbf{X}^{(\text{train})}, \mathbf{y} = \mathbf{y}^{(\text{train})}$) only. Hope that cost on test data is small.

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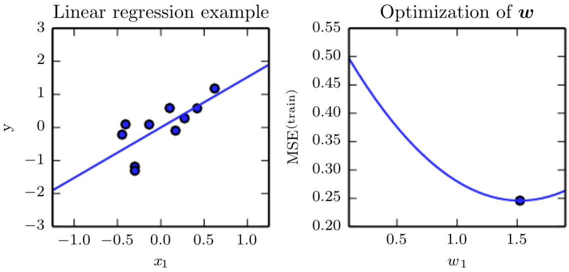

- *Left*: Data points, and the linear function $y = w_1 x$ that approximates them best
- *Right*: Mean squared error (MSE) depending on w_1
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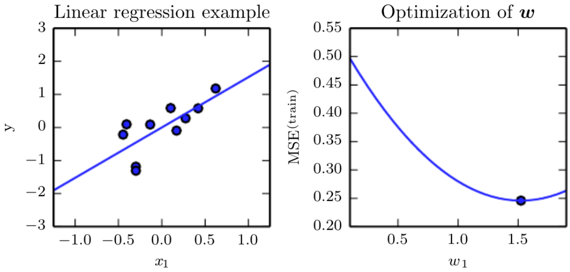

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Nearest Neighbor Classification

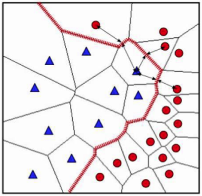
- Consider appropriate distance measure

$$D : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}_+ \quad (8)$$

- For unknown data point $\mathbf{x}$, determine the closest given data point

$$\mathbf{x}_{i*} := \text{argmin}_i (D(\mathbf{x}, \mathbf{x}_i)) \quad (9)$$

- Predict label of $\mathbf{x}$ as y_{i*}



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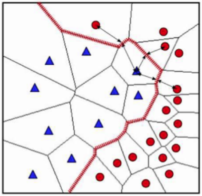


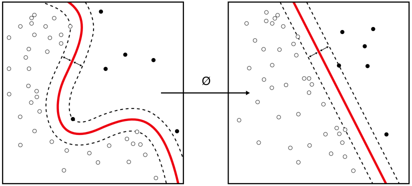
Support Vector Machines

- *Realization*: From (7), write

$$\mathbf{w}^T\mathbf{x} = \sum_{i=1}^{m} \alpha_i \mathbf{x}^T\mathbf{x}_i = \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle \tag{10}$$

- Replace $\langle ., . \rangle$ by different *kernel* (i.e. scalar product) $k(., .)$, that is by computing $\langle \phi(.), \phi(.) \rangle$ for appropriate ϕ

☞ Seek α's to maximize margin: still easy to optimize both for regression and classification!



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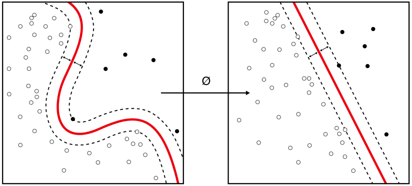

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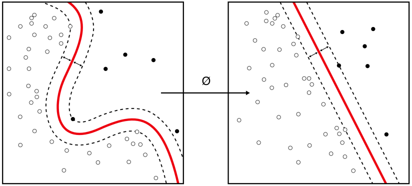
- Replace $\langle ., . \rangle$ by different *kernel* (i.e. scalar product) $k(., .)$, that is by computing $\langle \phi(.), \phi(.) \rangle$ for appropriate ϕ

☞ Seek α's to maximize margin: still easy to optimize both for regression and classification!



General / Further Reading

Literature

- Deep Learning, Chapter 5:
  https://www.deeplearningbook.org/