Machine learning: lecture 7

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Topics

- Regularization cont'd
  - regularized logistic regression
  - empirical vs. expected loss
- Support vector machine (part 1)
  - discrimination, "optimal" hyperplane
  - optimization via Lagrange multipliers

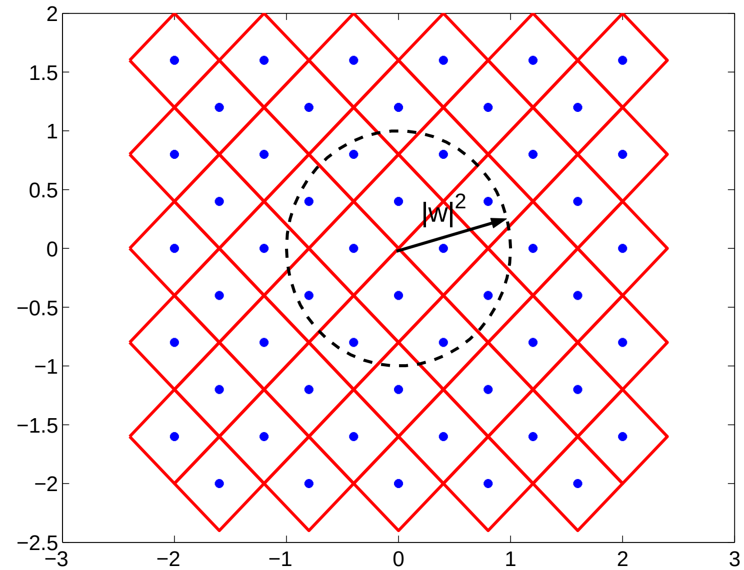
Review: "choices" in logistic regression

- Simple logistic regression model

$$P(y = 1|x, \mathbf{w}) = g(w_0 + w_1 x)$$

parameterized by $\mathbf{w} = (w_0, w_1)$. We assume that $x \in [-1, 1]$, i.e., that the inputs remain bounded.

- We can now divide the parameter space into regions with centers $\mathbf{w}_1, \mathbf{w}_2, \ldots$ such that the predictions of any $\mathbf{w}$ (for any $x \in [-1, 1]$) are close to those of one of the centers:

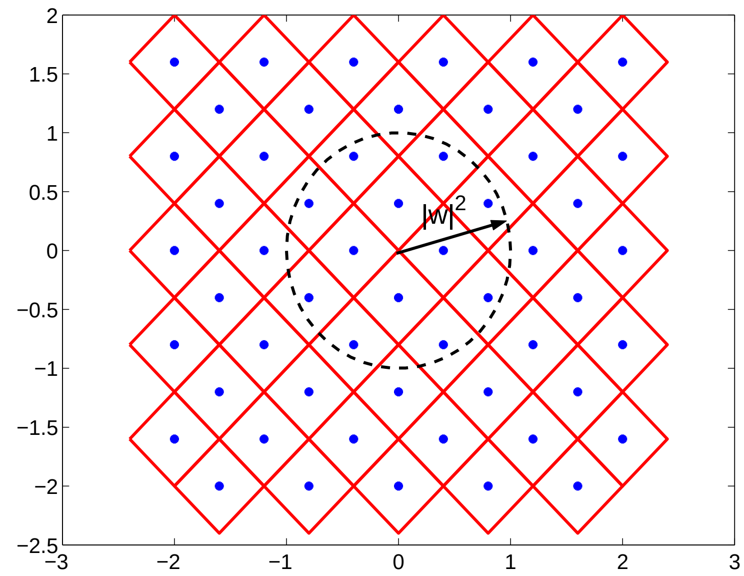


$$|\log P(y = 1|x, \mathbf{w}) - \log P(y = 1|x, \mathbf{w}_j)| \leq \epsilon$$

Review: regularized logistic regression

- We can regularize by imposing a penalty in the estimation criterion that encourages $\|\mathbf{w}\|$ to remain small.

  Maximum penalized likelihood



$$l(D; \mathbf{w}, \lambda) = \sum_{i=1}^{n} \log P(y_i | \mathbf{x}_i, \mathbf{w}) - \frac{\lambda}{2} \|\mathbf{w}\|^2$$

  where larger values of λ impose stronger regularization.

- More generally, we can assign penalties based on prior distributions over the parameters, i.e., add $\log P(\mathbf{w})$ in the log-likelihood criterion.

Effect of available "choices"

- We'd like the empirical loss of our parameter estimate $\hat{\mathbf{w}}$ to be close to its expected loss

  Example: m effective parameter choices

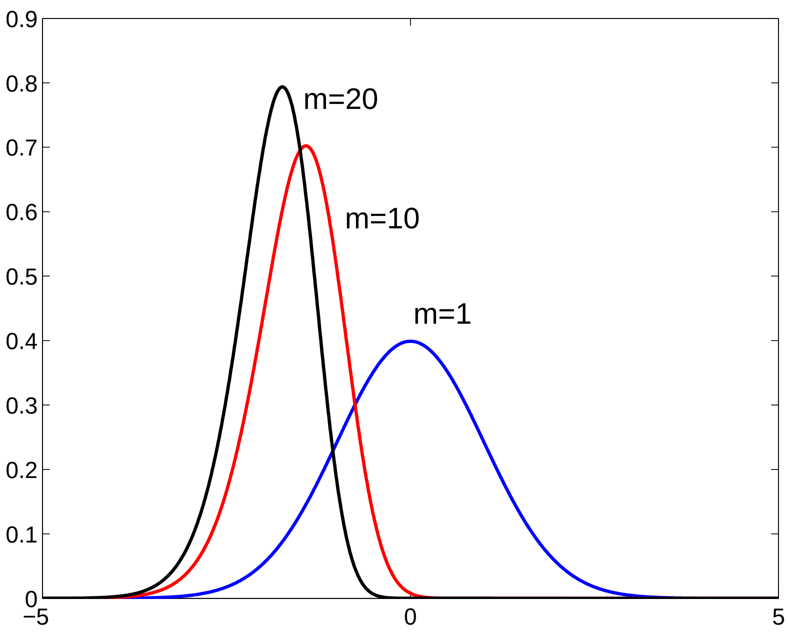
$$
\begin{aligned}
L_n(\mathbf{w}_k) &= \frac{1}{n}\sum_{i=1}^{n} \mathrm{Loss}(y_i, f(\mathbf{x}_i, \mathbf{w}_k)), \quad k = 1, \ldots, m \\
L_n(\hat{\mathbf{w}}) &= \min_i \{\, L_n(\mathbf{w}_i) \,\}
\end{aligned}
$$

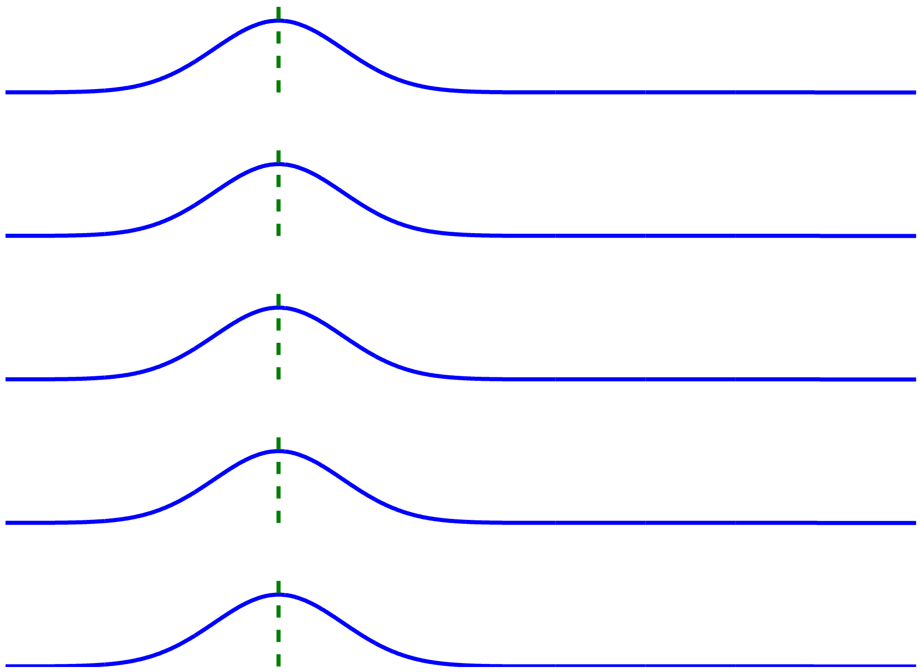
Empirical vs expected loss

- How is $\min_i \{ L_n(\mathbf{w}_i) \}$ distributed in the simple case where each

$$L_n(\mathbf{w}_k) \;=\; \frac{1}{n}\sum_{i=1}^{n} \mathrm{Loss}(y_i, f(\mathbf{x}_i, \mathbf{w}_k)),$$

is a zero mean Gaussian?





Topics

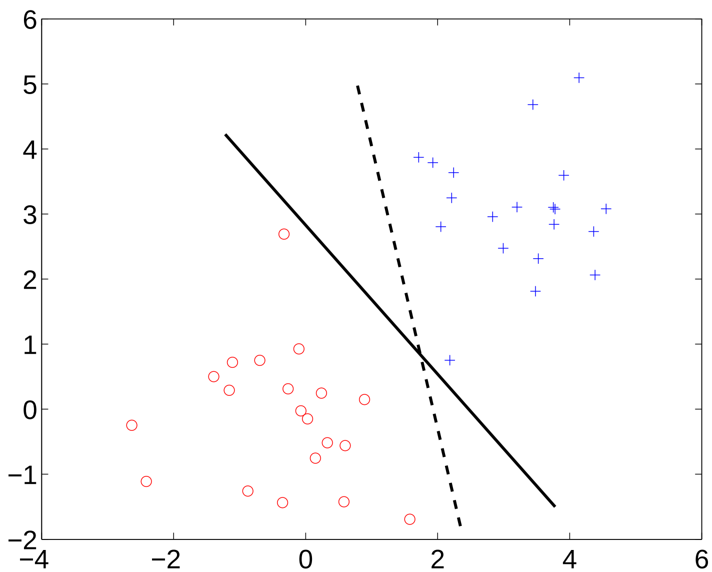
- Support vector machine
  - discrimination, “optimal” hyperplane
  - optimization via Lagrange multipliers
  - kernel function

Discriminative (non-probabilistic) classification

- Consider a binary classification task with $y = \pm 1$ labels (not $0/1$ as before). When the training examples are *linearly separable* we can set the parameters of a linear classifier so that all the training examples are classified correctly:

$$y_i \left[w_0 + \mathbf{w}^T \mathbf{x} \right] > 0, \;\; i = 1, \ldots, n$$

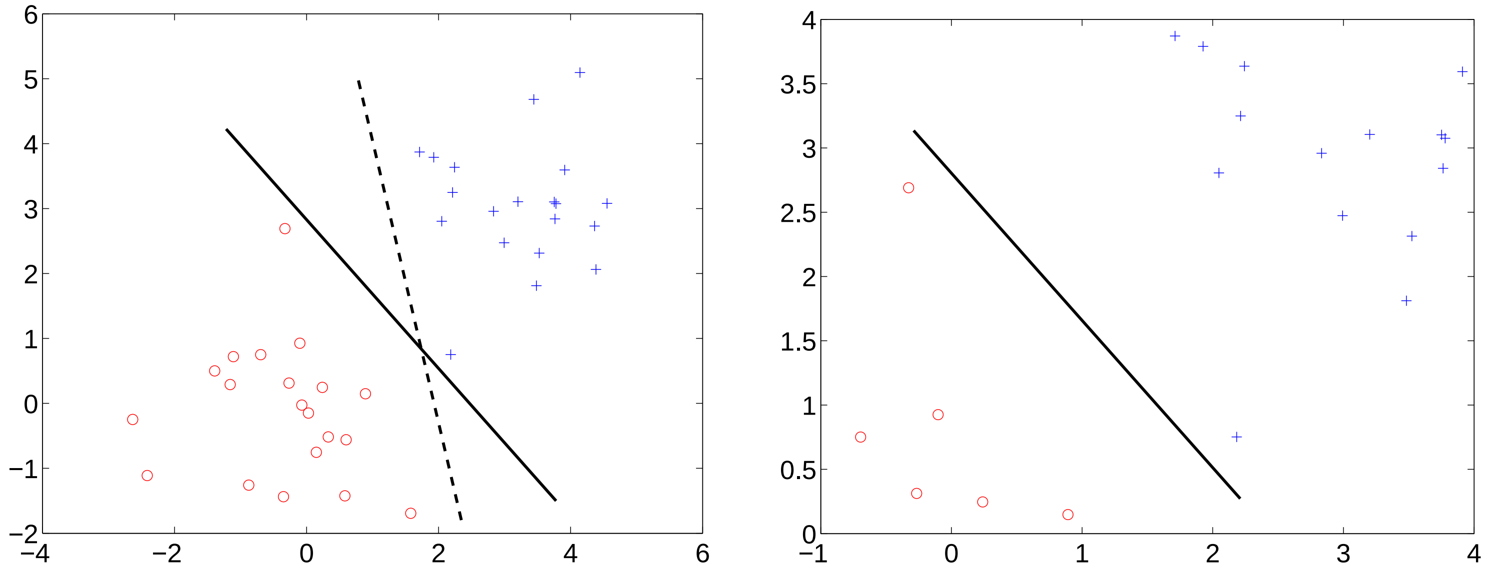
The label we predict for each example is given by the sign of the linear function $w_0 + \mathbf{w}^T\mathbf{x}$.



Classification and margin

- We can try to find a unique solution by requiring that the training examples are classified correctly with a non-zero "margin"

$$y_i \left[w_0 + \mathbf{w}^T \mathbf{x}_i \right] - 1 \geq 0, \; i = 1, \ldots, n$$



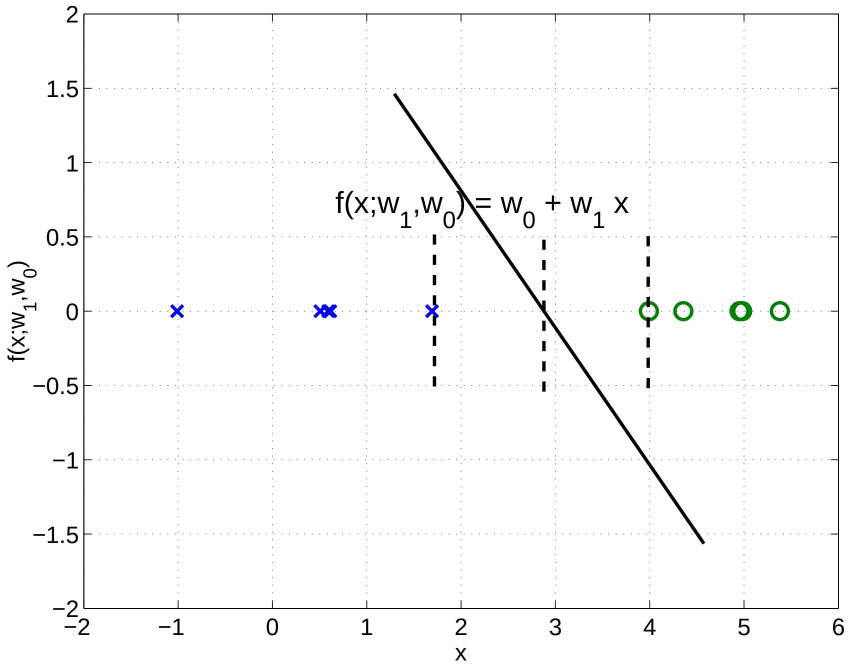
The margin should be defined in terms of the distance from the boundary to the examples rather than based on the value of the linear function.

Redefining margin

- One dimensional example: $f(x; w_1, w_0) = w_0 + w_1 x$.

  Relevant constraints:

$$\begin{aligned} 1\,[w_0 + w_1 x^+] - 1 &\geq 0 \\ -1\,[w_0 + w_1 x^-] - 1 &\geq 0 \end{aligned}$$



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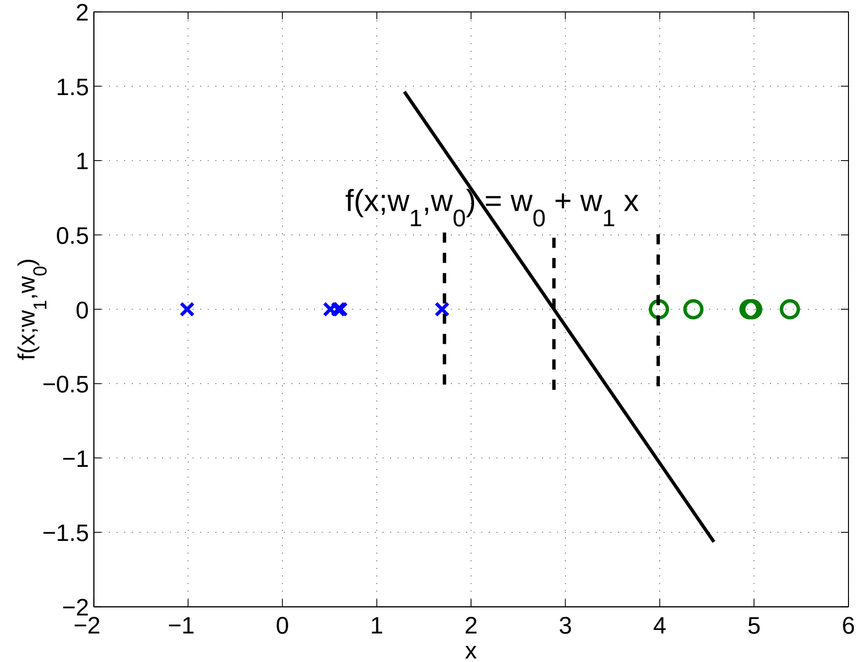
By adding the two inequalities we get

$$\begin{aligned} w_1(x^+ - x^-) - 2 &\geq 0 \\ \underbrace{|x^- - x^+|/2}_{\text{max margin}} &\geq \frac{1}{|w_1|} \end{aligned}$$



- We get maximum margin separation by minimizing $|w_1|$

Support vector machine

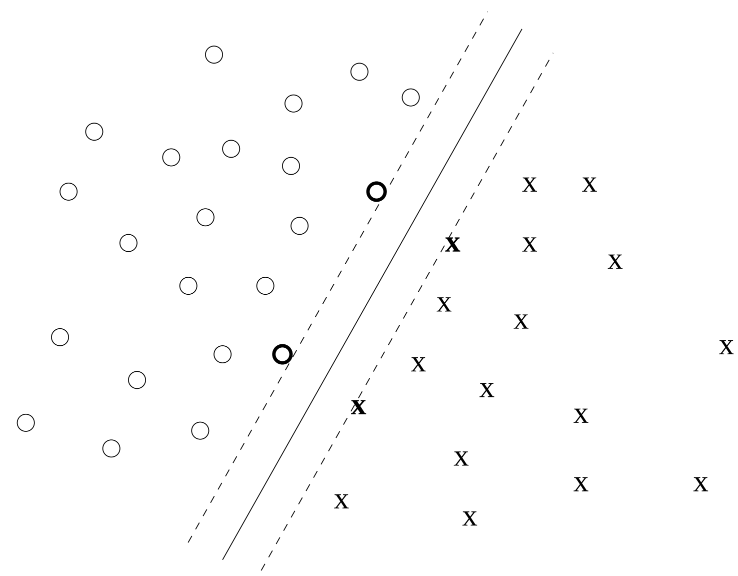
- We minimize a regularization penalty

$$\|\mathbf{w}\|^2/2 = \mathbf{w}^T\mathbf{w}/2 = \sum_{j=1}^{d} w_i^2/2$$

subject to the classification constraints

$$y_i\left[w_0 + \mathbf{w}^T\mathbf{x}_i\right] - 1 \geq 0, \quad i = 1, \ldots, n$$

- The attained margin is now given by $1/\|\mathbf{w}\|$
- Only a few of the classification constraints are relevant $\Rightarrow$ support vectors



Support vector machine cont'd

- We find the optimal setting of $\{w_0, \mathbf{w}\}$ by introducing *Lagrange multipliers* $\alpha_i \geq 0$ for the inequality constraints
- We *minimize*

$$J(\mathbf{w}, w_0, \alpha) = \|\mathbf{w}\|^2/2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left[w_0 + \mathbf{w}^T \mathbf{x}_i \right] - 1 \right)$$

with respect to $\mathbf{w}, w_0$. $\{\alpha_i\}$ ensure that the classification constraints are indeed satisfied.

For fixed $\{\alpha_i\}$

$$\frac{\partial}{\partial \mathbf{w}} J(\mathbf{w}, w_0, \alpha) = \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0$$

$$\frac{\partial}{\partial w_0} J(\mathbf{w}, w_0, \alpha) = -\sum_{i=1}^{n} \alpha_i y_i = 0$$

Solution

- Substituting the solution $\mathbf{w} = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i$ back into the objective leaves us with the following (dual) optimization problem over the Lagrange multipliers:
  We *maximize*

  $$J(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

  subject to the constraints

  $$\alpha_i \geq 0, \quad i = 1, \ldots, n, \quad \sum_{i=1}^n \alpha_i y_i = 0$$

  (For non-separable problems we have to limit $\alpha_i \leq C$)

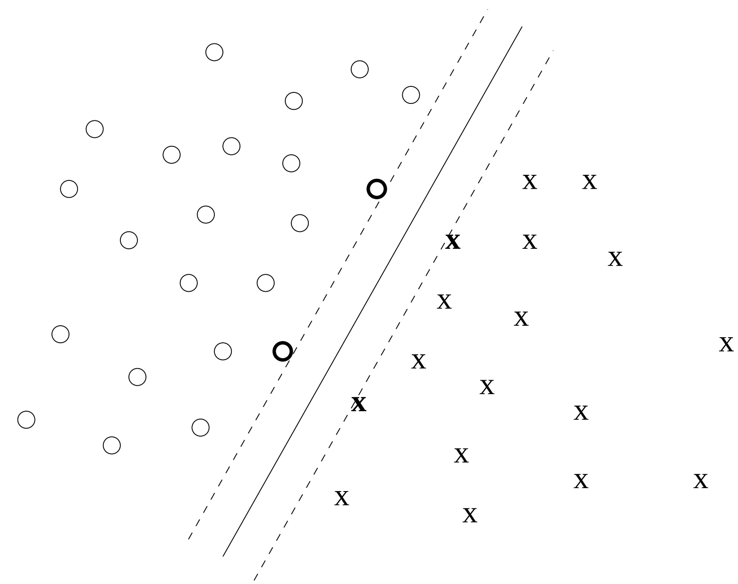
- This is a *quadratic programming problem*

Support vector machines

- Once we have the Lagrange multipliers $\{\hat{\alpha}_i\}$, we can reconstruct the parameter vector $\hat{\mathbf{w}}$ as a weighted combination of the training examples:

$$\hat{\mathbf{w}} = \sum_{i=1}^{n} \hat{\alpha}_i y_i \mathbf{x}_i$$

  where the "weight" $\hat{\alpha}_i = 0$ for all but the *support vectors* (SV)



- The decision boundary has an interpretable form

$$\hat{\mathbf{w}}^T\mathbf{x} + \hat{w}_0 = \sum_{i \in SV} \hat{\alpha}_i \, y_i \, (\mathbf{x}_i^T \mathbf{x}) + \hat{w}_0 = f(\mathbf{x}; \hat{\alpha}, \hat{w}_0)$$

Interpretation of support vector machines

- To use support vector machines we have to specify only the inner products (or *kernel*) between the examples $(\mathbf{x}_i^T \mathbf{x})$
- The weights $\{\alpha_i\}$ associated with the training examples are solved by enforcing the classification constraints.

  $\Rightarrow$ sparse solution

- We make decisions by comparing each new example $\mathbf{x}$ with **only** the support vectors $\{\mathbf{x}_i\}_{i \in SV}$:

$$\hat{y} = \operatorname{sign}\left(\sum_{i \in SV} \hat{\alpha}_i \, y_i \, (\mathbf{x}_i^T \mathbf{x}) + \hat{w}_0 \right)$$