Support Vector Machines (SVM)

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But the maximum margin hyperplane generalizes the best to new data

- According to computational learning theory
- Also known as statistical learning theory
- We won't get into the details of that
- Recall from the perceptron convergence proof
  - We assumed the existance of a best hyperplane $\mathbf{w}_0$
  - Which provided the maximum margin α
  - Such that $d_p \mathbf{w}_0^T \mathbf{x}_p \leqslant \alpha$ for all training points p
- The SVM actually finds this hyperplane

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Maximum margin problem

- Given a set of data from two classes $\{\mathbf{x}_p, d_p\}$
  - $\mathbf{x}_p \in \mathbb{R}^D$ and $d_p \in \{-1, 1\}$
  - Assume the classes are linearly separable for now
- Find the hyperplane that separates them
  - with maximum margin
- Equation of general linear discriminant function

$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

- Find $\mathbf{w}$ and b that give maximum margin
- How can we quantify margin?

$\mathbf{w}$ is perpendicular to the hyperplane, b defines its distance from the origin

$\mathbf{w}$ is perpendicular to the hyperplane

- Consider two points on the hyperplane $\mathbf{x}_A$ and $\mathbf{x}_B$
- Then $y(\mathbf{x}_A) = y(\mathbf{x}_B) = 0$ by definition
- So $0 = y(\mathbf{x}_A) - y(\mathbf{x}_B) = \mathbf{w}^T(\mathbf{x}_A - \mathbf{x}_B)$
- $\mathbf{x}_A - \mathbf{x}_B$ is a vector pointing along the hyperplane
- So $\mathbf{w}$ is perpendicular to the hyperplane

b defines the hyerplane's distance from the origin

- Consider a general point $\mathbf{x}$
- Its distance to the origin is $D = \dfrac{\mathbf{w}^T x}{||\mathbf{w}||}$
- If $\mathbf{x}$ is on the hyperplane, then $y(\mathbf{x}) = 0$
  - So $\mathbf{w}^T x = -b$
- So the distance from the hyperplane to the origin is

$$D = -\frac{b}{||\mathbf{w}||}$$

$\mathbf{w}$ is perpendicular to the hyperplane, b defines its distance from the origin

The distance from point $\mathbf{x}$ to the hyperplane is $y(\mathbf{x})/||\mathbf{w}||$

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- Consider a point $\mathbf{x}$ and its projection onto the hyperplane $\mathbf{x}_\perp$ so that $\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||}$
- We want to find r, the distance to the hyperplane
- Multiply both sides by $\mathbf{w}^T$ and add b

$$\mathbf{w}^T\mathbf{x} + b = \mathbf{w}^T\mathbf{x}_\perp + b + r\frac{||\mathbf{w}||^2}{||\mathbf{w}||}$$

$$y(\mathbf{x}) = y(\mathbf{x}_\perp) + r||\mathbf{w}||$$

$$r = \frac{y(\mathbf{x})}{||\mathbf{w}||}$$

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- The margin is defined as

$$\alpha = \min_p d_p \frac{y(\mathbf{x}_p)}{||\mathbf{w}||}$$
$$= \frac{1}{||\mathbf{w}||} \min_p d_p y(\mathbf{x}_p)$$

- We want to find $\mathbf{w}$ and that maximize the margin $\text{argmax}_{\mathbf{w},b} \frac{1}{||\mathbf{w}||} \min_p d_p y(\mathbf{x}_p)$
- Solving this problem is hard as it is written

We are free to choose a rescaling of $\mathbf{w}$

- If we replace $\mathbf{w}$ by $a\mathbf{w}$ and b with ab
- Then the margin is unchanged

$$\min_p d_p \frac{a\mathbf{w}^T\mathbf{x}_p + ab}{a||\mathbf{w}||} = \min_p d_p \frac{\mathbf{w}^T\mathbf{x}_p + b}{||\mathbf{w}||}$$

- So choose a such that $\min_p d_p(a\mathbf{w}^T\mathbf{x}_p + ab) = 1$
- Which means that for all points

$$d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$$

Maximum margin constrained optimization problem

- Then the maximum margin optimization becomes

$$\begin{aligned}&\mathrm{argmax}_{\mathbf{w},b}\frac{1}{||\mathbf{w}||}\min_p d_p y(\mathbf{x}_p)\\&=\mathrm{argmax}_{\mathbf{w},b}\frac{1}{||\mathbf{w}||}\end{aligned}$$

- With the constraints $d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$

Maximum margin constrained optimization problem

- Which is equivalent to $\mathrm{argmin}_{\mathbf{w},b}\ \frac{1}{2}||\mathbf{w}||^2$, subject to $d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$
- This is a well studied type of problem
  - A quadratic program with linear inequality constraints

Detour: Lagrange multipliers solve constrained optimization problems

- Want to maximize a function $f(x_1, x_2)$
- Subject to the equality constraint $g(x_1, x_2) = 0$
- Could solve $g(x_1, x_2) = 0$ for x_1 in terms of x_2
  - But that is hard to do in general (i.e., on computers)
- Or could use Lagrange multipliers
  - Which are easier to use in general (i.e., on computers)

Lagrange multipliers with general $\mathbf{x}$

- In general, we can write

$$\max_x f(\mathbf{x}) \text{ subject to } g(\mathbf{x}) = 0$$

- Constraint $g(\mathbf{x}) = 0$ defines a $D-1$ dimensional surface for D dimensional $\mathbf{x}$

Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = x_1 + x_2 - 1 = 0$

Gradients of g and f are orthogonal to surface at solution point

Gradients of g and f are orthogonal to surface at maximum of f

- For g because on all points on the surface $g(\mathbf{x}) = 0$
- For f because if it wasn't, you could move along the surface in the direction of the gradient to find a better maximum
- Thus ∇f and ∇g are (anti-)parallel
- And there must exist a scalar λ such that

$$\nabla f + \lambda \nabla g = 0$$

The Lagrangian function captures the constraints on and on the gradients

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$$

- Setting gradient of L with respect to $\mathbf{x}$ to 0 gives

$$\nabla f + \lambda \nabla g = 0$$

- Setting partial of L with respect to λ to 0 gives

$$g(\mathbf{x}) = 0$$

- Thus stationary points of L solve the constrained optimization problem

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- So the Lagrangian function is

$$\begin{aligned} L(\mathbf{x}, \lambda) &= f(\mathbf{x}) + \lambda g(\mathbf{x}) \\ &= 1 - x_1^2 - x_2^2 + \lambda(x_1 + x_2 - 1) \end{aligned}$$

- The conditions for L to be stationary are

$$\begin{aligned} \partial L/\partial x_1 &= -2x_1 + \lambda = 0 \\ \partial L/\partial x_2 &= -2x_2 + \lambda = 0 \\ \partial L/\partial \lambda &= x_1 + x_2 - 1 = 0 \end{aligned}$$

- Can solve to find $\lambda = 1, x_1 = x_2 = \dfrac{1}{2}$

Lagrange multipliers can also be used with inequality constraints $g(\mathbf{x}) \geqslant 0$

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- Now two kinds of solutions:
- If $g(\mathbf{x}) > 0$, then the solution only depends on $f(\mathbf{x})$
  - Inside constraint surface with $\nabla f = 0$
  - Stationary point of $L(\mathbf{x}, \lambda)$ with $\lambda = 0$
  - Constraint $g(\mathbf{x})$ is said to be inactive
- If $g(x) = 0$, then same as before (with equality constraint)
  - On boundary of constraint surface with ∇f pointing out
  - Stationary point of $L(\mathbf{x}, \lambda)$ with $\lambda > 0$
  - Constraint $g(\mathbf{x})$ is said to be active

Lagrange multipliers can also be used with inequality constraints $g(\mathbf{x}) \geqslant 0$

- In either case, $\lambda g(\mathbf{x}) = 0$
- Thus maximizing $f(\mathbf{x})$ subject to $g(\mathbf{x}) \geqslant 0$ is obtained by optimizing $L(\mathbf{x}, \lambda)$ *w.r.t.* $\mathbf{x}$ and λ subject to

$$\begin{aligned} g(\mathbf{x}) &\geqslant 0 \\ \lambda &\geqslant 0 \\ \lambda g(\mathbf{x}) &= 0 \end{aligned}$$

- These are known as the Karush-Kuhn-Tucker (KKT) conditions

Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = x_1 + x_2 - 1 \geqslant 0$

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- So the Lagrangian function is

$$L(\mathbf{x}, \lambda) = 1 - x_1^2 - x_2^2 + \lambda(x_1 + x_2 - 1)$$

- The conditions for L to be stationary are

$$\begin{aligned} \partial L/\partial x_1 &= -2x_1 + \lambda = 0 \\ \partial L/\partial x_2 &= -2x_2 + \lambda = 0 \\ \partial L/\partial \lambda &= x_1 + x_2 - 1 = 0 \end{aligned}$$

- Can solve to find $\lambda = 1, x_1 = x_2 = \dfrac{1}{2}$
  - Which still satisfies KKT conditions

Example: Maximize $f(\mathbf{x}) = 1 - x_1^2 - x_2^2$ subject to $g(\mathbf{x}) = -x_1 - x_2 + 1 \geqslant 0$

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- So the Lagrangian function is

$$L(\mathbf{x}, \lambda) = 1 - x_1^2 - x_2^2 + \lambda(-x_1 - x_2 + 1)$$

- The conditions for L to be stationary are

$$\begin{aligned} \partial L/\partial x_1 &= -2x_1 - \lambda = 0 \\ \partial L/\partial x_2 &= -2x_2 - \lambda = 0 \\ \partial L/\partial \lambda &= x_1 + x_2 - 1 = 0 \end{aligned}$$

- Can solve to find $\lambda = -1$
  - which does not satisfy KKT condition $\lambda \geqslant 0$
- Instead use unconstrained solution $x_1 = x_2 = 0$
  - which does satisfy KKT conditions

Multiple constraints each get their own Lagrange multiplier

- Maximize $f(\mathbf{x})$ subject to $g_i(\mathbf{x}) = 0$ and $h_j(x) \geqslant 0$
- Leads to the Lagrangian function

$$L(\mathbf{x}, \lambda, \mu) = f(\mathbf{x}) + \sum_i \lambda_i g_i(\mathbf{x}) + \sum_j u_j h_j(\mathbf{x})$$

- Still solve for $\nabla L(\mathbf{x}, \lambda, \mu) = 0$
- Trickier in general to figure out which $h_j(\mathbf{x})$ constraints should be active

Minimizing $f(\mathbf{x})$ with an inequality constraint requires a slightly different Lagrange

- Minimize *w.r.t.* $\mathbf{x}$

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda g(\mathbf{x})$$

- Still subject to

$$g(\mathbf{x}) \geqslant 0$$

Summary of Lagrange multipliers with multiple inequality constraints

- Goal: maximize $f(\mathbf{x})$ subject to $g_i(\mathbf{x}) \geqslant 0$
- Write down Lagrangian function

$$L(\mathbf{x}, \lambda) = f(x) + \sum_i \lambda_i g_i(\mathbf{x})$$

- Find points where $\nabla L(\mathbf{x}, \lambda) = 0$
- Keep points that satisfy constraints $g_x(\mathbf{x}) \geqslant 0$
- Figure out which KKT conditions should be active
  - Don't need to try all 2^I combinations for SVMs
  - Because $f(\mathbf{x})$ and $g(\mathbf{x})$ form a "quadratic program"

Back to SVMs: Maximum margin solution is a fixed point of the Lagrangian function

- Recall, the maximum margin hyperplane is $\text{argmin}_{\mathbf{w},b} \frac{1}{2}||\mathbf{w}||^2$ subject to $d_p(\mathbf{w}^T\mathbf{x}_p + b) \geqslant 1$
  - Minimization of a quadratic function subject to multiple linear inequality constraints
- Will use Lagrange multipliers, a_p, to write Lagrangian function

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}||\mathbf{w}||^2 - \sum_p a_p(d_p(\mathbf{w}^T\mathbf{x}_p + b) - 1)$$

- Note that $\mathbf{x}_p$ and d_p are fixed for the optimization

Thank you!