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COMPSCI 689
Lecture 11: Lagrangian Duality and Kernel SVMs

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The Lagrangian

- The fundamental tool for analyzing constrained optimization problems is the Lagrangian function.

- Given an objective function $f(\mathbf{x})$ and a set of equality and inequality constraint functions $c_i(\mathbf{x}) = 0$ for $i \in \mathcal{E}$ and $c_i(\mathbf{x}) \geq 0$ for $i \in \mathcal{I}$, the Lagrangian is the function:

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{i \in \mathcal{I}} \lambda_i c_i(\mathbf{x}) - \sum_{i \in \mathcal{E}} \lambda_i c_i(\mathbf{x})$$

- The new variables λ_i are referred to as *Lagrange Multipliers*.

- The KKT conditions specify the necessary first-order conditions for $\mathbf{x}_*$ to be the constrained minimizer of $f(\mathbf{x})$ in terms of the Lagrangian $\mathcal{L}(\mathbf{x}, \lambda)$.

The KKT Conditions

- Suppose that $\mathbf{x}_*$ is a solution to a constrained optimization problem with Lagrangian $\mathcal{L}(\mathbf{x}, \lambda)$ and constraints $c_i(\mathbf{x}) = 0$ for $i \in \mathcal{E}$ and $c_i(\mathbf{x}) \geq 0$ for $i \in \mathcal{I}$. Then there exists a λ_* such that:

$$
\begin{aligned}
\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}_*, \lambda_*) &= 0 \\
c_i(\mathbf{x}_*) &= 0 \text{ for all } i \in \mathcal{E} \\
c_i(\mathbf{x}_*) &\geq 0 \text{ for all } i \in \mathcal{I} \\
\lambda_{i*} &\geq 0 \text{ for all } i \in \mathcal{I} \\
\lambda_{i*}c_i(\mathbf{x}_*) &= 0 \text{ for all } i \in \mathcal{I}
\end{aligned}
$$

- For convex problems, if $(\mathbf{x}_*, \lambda_*)$ satisfy the KKT conditions, then $\mathbf{x}_*$ is the global constrained optimum.

Method of Lagrange Multipliers

- If we only have equality constraints, to find a point that satisfies the KKT conditions, we identify and analyze the stationary points of the Lagrangian by solving the Lagrangian gradient system:

$$\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}, \lambda) = 0$$
$$\nabla_{\lambda}\mathcal{L}(\mathbf{x}, \lambda) = 0$$

- We identify all values of $\mathbf{x}$, and λ satisfying the above equations, plug the values of $\mathbf{x}$ into $f(\mathbf{x})$ and determine the minimizer.

- This is called the method of Lagrange multipliers.

What About Inequality Constraints?

- Even linear inequality constraints can make convex optimization problems harder to solve.

- There exist specialized algorithms for solving many different kinds of convex optimization problems including linear programs (LPs), quadratic programs (QPs), second-order cone programs (SOCPs), etc. that include constraints.

- A general strategy in optimization is to transform a problem for which there are no convenient solution methods into a form where the problem can be more easily solved or that exposes additional properties (see SVC margin to hinge loss transformation).

- One often useful transformation of a convex optimization problem with inequality constraints is the *Lagrange Dual*.

The Lagrange Dual

- Suppose we have a constrained optimization problem with objective function $f(x)$ and constraint functions $c_i(\mathbf{x}) \geq 0$ and $c_i(\mathbf{x}) = 0$. We can form the Lagrangian as shown below:

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}) - \sum_{i \in \mathcal{E}} \lambda_i c_i(\mathbf{x}) - \sum_{i \in \mathcal{I}} \lambda_i c_i(\mathbf{x})$$

- The Lagrange dual function of the original optimization problem is:

$$q(\lambda) = \min_{\mathbf{x} \in \mathcal{X}} \mathcal{L}(\mathbf{x}, \lambda)$$

- This function is subject to the constraints $\lambda_i \geq 0$ for $i \in \mathcal{I}$.

Deriving the Lagrange Dual

1. Given $f(\mathbf{x})$ and constraint functions $c_i(\mathbf{x})$, form the Lagrangian $\mathcal{L}(\mathbf{x}, \lambda)$.

2. Derive the gradient $\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda)$.

3. Form the stationary equations $\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda) = 0$.

4. The stationary equations will yield relationships between primary parameters and Lagrange multipliers that hold when $\mathbf{x}_* = \arg\min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda)$.

5. These relationships can be used to eliminate the primary parameters from the Lagrangian, yielding $q(\lambda) = \mathcal{L}(\mathbf{x}_*, \lambda)$ and possibly some additional equality constraints.

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Properties of the Lagrange Dual

- For any value of λ satisfying the constraints, $q(\lambda)$ provides a lower bound on the primal objective function value $f(\mathbf{x}_*)$ at the constrained minimizer $\mathbf{x}_*$. In other words: $f(\mathbf{x}_*) \geq q(\lambda)$.

- If there exists a λ_* such that $f(\mathbf{x}_*) = q(\lambda_*)$, then *strong duality* is said to hold. Otherwise, *weak duality* holds.

- Strong duality typically holds for convex optimization problems with convex constraints.

Properties of Strong Duality

- When strong duality holds, **minimizing** the primal objective function $f(\mathbf{x})$ with respect to $\mathbf{x}$ subject to the primal constraints is exactly equivalent to **maximizing** the Lagrange dual function $q(\lambda)$ with respect to λ subject to the dual constraints [1]:

$$\lambda_* = \arg\max_\lambda q(\lambda)$$
$$\text{s.t.} \quad \lambda_i \geq 0 \; ... \; \text{for } i \in \mathcal{I}$$

- Finally, it is also possible to recover the optimal value of $\mathbf{x}_*$ from λ_*, typically using relationships between them derived in the process of forming the Lagrange dual from the primal.

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[1] Note that additional equality constraints may sometimes be produced in the process of forming the dual, and these also need to be included in the dual problem formulation

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The SVC Primal Optimization Problem

- Recall that the constrained version of the SVC optimization problem has the form shown below.

$$
\arg\min_{\mathbf{w},b,\epsilon} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n
$$
$$
\text{s.t. } \forall n \ \ y_n(\mathbf{x}_n\mathbf{w} + b) \geq 1 - \epsilon_n
$$
$$
\forall n \ \ \epsilon_n \geq 0.
$$

- This problem has a convex objective with convex constraints. We will derive its Lagrange dual.

Lagrangian

$$\arg\min_{\mathbf{w},b,\epsilon} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n$$
$$\text{s.t. } \forall n \ \ y_n(\mathbf{x}_n\mathbf{w}+b) \geq 1-\epsilon_n$$
$$\forall n \ \ \epsilon_n \geq 0.$$

$$\mathcal{L}(\mathbf{w},b,\epsilon,\alpha,\beta) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n$$
$$- \sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n\mathbf{w}+b)+\epsilon_n-1)$$
$$\text{s.t. } \forall n \ \ \alpha_n \geq 0, \beta_n \geq 0$$

Minimizing wrt w

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n$$
$$- \sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n\mathbf{w} + b) + \epsilon_n - 1)$$
$$\text{s.t. } \forall n \ \ \alpha_n \geq 0, \beta_n \geq 0$$

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \mathbf{w} - \sum_{n=1}^{N}\alpha_n y_n \mathbf{x}_n^T = 0$$
$$\mathbf{w} = \sum_{n=1}^{N}\alpha_n y_n \mathbf{x}_n^T$$

Minimizing wrt b

$$
\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n
$$
$$
-\sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n\mathbf{w} + b) + \epsilon_n - 1)
$$
$$
\text{s.t. } \forall n \;\; \alpha_n \geq 0, \beta_n \geq 0
$$

$$
\nabla_b\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = -\sum_{n=1}^{N}\alpha_n y_n = 0
$$
$$
\sum_{n=1}^{N}\alpha_n y_n = 0
$$

Minimizing wrt ϵ

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n$$

$$-\sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n\mathbf{w} + b) + \epsilon_n - 1)$$

$$\text{s.t. } \forall n \;\; \alpha_n \geq 0, \beta_n \geq 0$$

$$\nabla_{\epsilon_n}\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = C - \beta_n - \alpha_n = 0$$

$$\alpha_n + \beta_n = C$$

Substituting into Lagrangian

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n$$
$$- \sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n\mathbf{w} + b) + \epsilon_n - 1)$$

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2}\|\sum_{m=1}^{N}\alpha_m y_m \mathbf{x}_m^T\|_2^2 + C\sum_{n=1}^{N}\epsilon_n - \sum_{n=1}^{N}\beta_n\epsilon_n$$
$$- \sum_{n=1}^{N}\alpha_n(y_n(\mathbf{x}_n(\sum_{m=1}^{N}\alpha_m y_m \mathbf{x}_m^T) + b) + \epsilon_n - 1)$$

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Expanding Terms

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2} \| \sum_{m=1}^{N} \alpha_m y_m \mathbf{x}_m^T \|_2^2 + C \sum_{n=1}^{N} \epsilon_n - \sum_{n=1}^{N} \beta_n \epsilon_n$$
$$- \sum_{n=1}^{N} \alpha_n (y_n (\mathbf{x}_n (\sum_{m=1}^{N} \alpha_m y_m \mathbf{x}_m^T) + b) + \epsilon_n - 1)$$

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T + C \sum_{n=1}^{N} \epsilon_n - \sum_{n=1}^{N} \beta_n \epsilon_n$$
$$- \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T - \sum_{n=1}^{N} \alpha_n (y_n b + \epsilon_n - 1)$$

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Simplifying I

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T + C \sum_{n=1}^{N} \epsilon_n - \sum_{n=1}^{N} \beta_n \epsilon_n$$
$$- \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T - \sum_{n=1}^{N} \alpha_n (y_n b + \epsilon_n - 1)$$

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = -\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T + \sum_{n=1}^{N} (\alpha_n + \beta_n) \epsilon_n$$
$$- \sum_{n=1}^{N} \beta_n \epsilon_n - \sum_{n=1}^{N} \alpha_n (y_n b + \epsilon_n - 1)$$

Simplifying II

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = -\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T + \sum_{n=1}^{N} (\alpha_n + \beta_n) \epsilon_n$$
$$- \sum_{n=1}^{N} \beta_n \epsilon_n \ - \sum_{n=1}^{N} \alpha_n (y_n b + \epsilon_n - 1)$$

$$\mathcal{L}(\mathbf{w}, b, \epsilon, \alpha, \beta) = -\frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n \mathbf{x}_m^T \ + \sum_{n=1}^{N} \alpha_n$$

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Constraint Simplification

$$\alpha_n \geq 0$$
$$\beta_n \geq 0$$
$$\sum_{n=1}^{N} \alpha_n y_n = 0$$
$$\alpha_n + \beta_n = C$$

$$\sum_{n=1}^{N} \alpha_n y_n = 0$$
$$0 \leq \alpha_n \leq C$$

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The SVC Dual Optimization Problem

- The SVC dual optimization problem is given below where we have used α_n as the Lagrange multipliers.

$$\arg\max_{\boldsymbol{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m \mathbf{K}_{nm}$$

$$\text{s.t. } \forall n \ \ 0 \leq \alpha_n \leq C$$

$$\sum_{n=1}^{N} \alpha_n y_n = 0$$

- The matrix $\mathbf{K}$ that appears in the objective contains the inner products between all pairs of training data vectors: $\mathbf{K}_{nm} = \mathbf{x}_n \mathbf{x}_m^T$. The matrix $\mathbf{K}$ is thus positive semi-definite and the optimization problem is maximizing a concave function.

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SVC Dual Predictions

- Given the value of $\boldsymbol{\alpha}$, we can make predictions as follows:

$$f_{svm}(\mathbf{x}) = \sum_{n=1}^{N} y_n \alpha_n \mathbf{x}_n \mathbf{x}^T + b$$

- There are a number of ways to derive the optimal b from the KKT conditions and an optimal $\boldsymbol{\alpha}$. One approach is to use the equation below where $\mathcal{S}$ is the set of data points satisfying $0 < \alpha_n < C$:

$$b = \frac{1}{|\mathcal{S}|} \sum_{n \in \mathcal{S}} \left(y_n - \sum_{m \in \mathcal{S}} y_m \alpha_m \mathbf{x}_m \mathbf{x}_n^T \right)$$

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Support Vector Property

- The above results show that only the data points for which $\alpha_n > 0$ actually participate in defining the learned model and making predictions.

- The data points for which $\alpha_n > 0$ are the support vectors. For the linearly separable case, these are the data cases on the margin. For the non-separable case, the are the data points on, within and on the wrong side of the margin.

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Basis Expansion

- One of the important applications of the SVC dual problem is constructing non-linear classifiers.

- Recall that we can make a linear model non-linear by introducing a basis function expansion $\phi(\mathbf{x})$.

- Plugging this into the dual, we obtain the learning problem shown below where the only change is $\mathbf{K}_{nm} = \phi(\mathbf{x}_n)\phi(\mathbf{x}_m)^T$.

$$\arg\max_{\boldsymbol{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m \mathbf{K}_{nm}$$

$$\text{s.t. } \forall n \ \ 0 \leq \alpha_n \leq C$$

$$\sum_{n=1}^{N} \alpha_n y_n = 0$$

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Kernels

- The only requirement for the optimization problem to be well-defined is for the matrix $\mathbf{K}$ to be positive semi-definite.

- An alternative to using an explicit basis expansion is to use a kernel function $\mathcal{K}(\mathbf{x}, \mathbf{x}')$ that is guaranteed to generate a positive definite matrix $\mathbf{K}$ given any collection of data vectors $\mathbf{x}_n$. Such a kernel function is referred to as a *Mercer* kernel.

- In the learning problem, instead of setting $\mathbf{K}_{nm} = \phi(\mathbf{x}_n)\phi(\mathbf{x}_m)^T$, we set $\mathbf{K}_{nm} = \mathcal{K}(\mathbf{x}_n, \mathbf{x}_m)$.

- The prediction function becomes:

$$f_{svm}(\mathbf{x}) = \sum_{n=1}^{N} y_n \alpha_n \mathcal{K}(\mathbf{x}_n, \mathbf{x}) + b$$

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Example: Kernels

- Linear Kernel: $\mathcal{K}(\mathbf{x}', \mathbf{x}) = \mathbf{x}'\mathbf{x}^T$

- Polynomial Kernel: $\mathcal{K}(\mathbf{x}', \mathbf{x}) = (1 + \mathbf{x}'\mathbf{x}^T)^B$

- Exponential (RBF) Kernel: $\mathcal{K}(\mathbf{x}', \mathbf{x}) = a \exp\left(-b\|\mathbf{x}' - \mathbf{x}\|_2^2\right)$

- ... and many more kernel functions, including for inputs that are not real-valued.

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Properties of Duals and Kernels

- The optimization problem remains concave when using kernels, but the decision function can be complex and non-linear.

- When there existis a kernel implementing a given basis expansion, the dual formulation results in a QP that scales with N while the primal results in a QP that scales with the size of the basis expansion.

- There exist kernel functions (like the RBF kernel) that do not correspond to finite-dimensional basis expansions that can be used exactly in the dual, but must be approximated to use in the primal.

Generalizing Kernelization

- Any convex supervised learning optimization problem with convex (or no constraints) has a similar dual to SVC and can usually be kernelized as well (linear regression, SVR, logistic regression, GLMs, etc.).

- However, only SVC and SVR have a direct sparsity property where we typically expect many dual variables to be zero.