SVAN 2016 Mini-Course

Stochastic Convex Optimization Methods in Machine Learning

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Coordinate Optimization vs. Stochastic Gradient

- Consider optimization problem:

$$\operatorname*{argmin}_{x \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(x).$$

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  - Fast convergence rate, but iterations must be d times cheaper than gradient method.
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  - Functions f_i can be non-smooth.
- SAG: update all x_i based on one example (and old versions of others):
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Motivation: Multi-Dimensional Polynomial Basis

- Recall using polynomial basis when we only have one features ($x_i \in \mathbb{R}$):

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- We can fit these models using a change of basis:

$$\text{If } X = \begin{bmatrix} 0.2 \\ -0.5 \\ 1 \\ 4 \end{bmatrix} \text{ then let } \Phi(X) = \begin{bmatrix} 1 & 0.2 & (0.2)^2 \\ 1 & -0.5 & (-0.5)^2 \\ 1 & 1 & (1)^2 \\ 1 & 4 & (4^2) \end{bmatrix},$$

and L2-regularized least squares solution is

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- How can we do this when we have a lot of features?

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- Approach 1: use polynomial basis for each variable:

$$X = \begin{bmatrix} 0.2 & 0.3 \\ 1 & 0.5 \\ -0.5 & -0.1 \end{bmatrix} \Rightarrow \Phi(X) = \begin{bmatrix} 1 & 0.2 & (0.2)^2 & 0.3 & (0.3)^2 \\ 1 & 1 & (1)^2 & 0.5 & (0.5)^2 \\ 1 & -0.5 & (-0.5)^2 & -0.1 & (-0.1)^2 \end{bmatrix}$$

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- But this is restrictve:
  - We should allow terms like $x_{i1}x_{i2}$ that depend on feature interactions.
  - But number of terms in X_{poly} would be huge:
    - Degree-5 polynomial basis has $O(d^5)$ terms:

$$x_{i1}^5, x_{i1}^4 x_{i2}, x_{i1}^4 x_{i3}, \ldots, x_{i1}^3 x_{i2}^2, x_{i1}^3 x_{i2}^2, \ldots, x_{i1}^3 x_{i2} x_{i3}, \ldots$$

- If n is not too big, we can do this efficiently using the kernel trick.

Equivalent Form of Ridge Regression

- Recall the L2-regularized least squares model,

$$\underset{w \in \mathbb{R}^d}{\text{argmin}} \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2.$$

- We showed that the solution is

$$w = (\underbrace{X^T X}_{d \text{ by } d} + \lambda I_d)^{-1} X^T y,$$

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  where I_d is the d by d identity matrix.
- An equivalent way to write the solution is:

$$w = X^T (\underbrace{X X^T}_{n \text{ by } n} + \lambda I_n)^{-1} y,$$

  by using a variant of the matrix inversion lemma.
- Computing w with this formula is faster if $n << d$:
  - since XX^T is n by n while $X^T X$ is d by d.

Predictions using Equivalent Form

- Given test data $\hat{X}$, we predict $\hat{y}$ using:

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- If we define $K = XX^T$ (Gram matrix) and $\hat{K} = \hat{X}X^T$, then we have

$$\hat{y} = \hat{K}(K + \lambda I_n)^{-1}y.$$

- Key observation behind kernel trick:
  - If we have the K and $\hat{K}$, we don't need the features.

Gram Matrix

- The Gram matrix K is defined by:

$$K = XX^T = \begin{bmatrix} — & x_1 & — \\ — & x_2 & — \\ & \vdots & \\ — & x_n & — \end{bmatrix} \begin{bmatrix} | & | & | \\ x_1 & x_2 & x_3 \\ | & | & | \end{bmatrix}$$

$$= \begin{bmatrix} x_1^T x_1 & x_1^T x_2 & \cdots & x_1^T x_n \\ x_2^T x_1 & x_2^T x_2 & \cdots & x_2^T x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^T x_1 & x_n^T x_2 & \cdots & x_n^T x_n \end{bmatrix}$$

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- K contains the inner products between all training examples.
- $\hat{K}$ contains the inner products between training and test examples.
  - If we can compute inner products $k(x_i, x_j) = x_i^T x_j$, we don't need x_i and x_j.

Polynomial Kernel

- Consider two examples x_i and x_j for a two-dimensional dataset:

$$x_i = (x_{i1}, x_{i2}), \quad x_j = (x_{j1}, x_{j2}).$$

- Consider a particular degree-2 basis ϕ:

$$\phi(x_i) = (x_{i1}^2, \sqrt{2}x_{i1}x_{i2}, x_{i2}^2).$$

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$$\begin{aligned}
\phi(x_i)^T\phi(x_j) &= \begin{bmatrix} x_{i1}^2 & \sqrt{2}x_{i1}x_{i2} & x_{i2}^2 \end{bmatrix} \phi(x_j) \\
&= x_{i1}^2x_{j1}^2 + 2x_{i1}x_{i2}x_{j1}x_{j2} + x_{i2}^2x_{j2}^2 \\
&= (x_{i1}x_{j1} + x_{i2}x_{j2})^2 \qquad \text{(completing the square)} \\
&= \left(\sum_{k=1}^{d} x_{ik}x_{jk}\right)^2 \\
&= (x_i^T x_j)^2.
\end{aligned}$$

Polynomial Kernel with Higher Degrees

- If we want all degree-4 "monomials", raise to 4^{th} power:

$$\phi(x_i)^T \phi(x_j) = (x_i^T x_j)^4,$$

where $\phi(x_i)$ is weighted version of $x_{i1}^4, x_{i1}^3 x_{i2}, x_{i1}^2 x_{i2}^2, x_{i1} x_{i2}^3, x_{i2}^4$.

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- If you want bias or lower-order terms like x_{i1}, add constant inside power:

$$(1 + x_i^T x_j)^2 = 1 + 2x_i^T x_j + (x_i^T x_j)^2$$

$$= \begin{bmatrix} 1 & 2x_{i1} & 2x_{i2} & x_{i1}^2 & \sqrt{2}x_{i1}x_{i2} & x_{i2}^2 \end{bmatrix} \begin{bmatrix} 1 \\ 2x_{j1} \\ 2x_{j2} \\ x_{j1}^2 \\ \sqrt{2}x_{j1}x_{j2} \\ x_{j2}^2 \end{bmatrix} = \phi(x_i)^T\phi(x_j),$$

- These formulas still work for any dimension of the x_i.

Kernel Trick

- Using polynomial basis of degree 'p' with the kernel trick:
  - Compute K and $\hat{K}$ which have elements:

$$k(x_i, x_j) = (1 + x_i^T x_j)^p, \quad \hat{k}(\hat{x}_i, x_j) = (1 + \hat{x}_i^T x_j)^p.$$

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- Kernel trick lets us fit regression models without explicit feature calculation:
  - Features may have exponential or infinite size.

Guasian-RBF Kernels

- The most common kernel is the Gaussian-RBF (or 'squared exponential') kernel,

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right).$$

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$$\begin{aligned} k(x_i, x_j) &= \exp(-x_i^2 + 2x_i x_j - x_j^2) \\ &= \exp(-x_i^2)\exp(2x_i x_j)\exp(-x_j^2), \end{aligned}$$

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  so we need $\phi(x_i) = \exp(-x_i^2)z_i$ where $z_i z_j = \exp(2x_i x_j)$.
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  - If we use that

$$\exp(2x_i x_j) = \sum_{k=0}^{\infty} \frac{2^k x_i^k x_j^k}{k!},$$

  then we obtain

$$\phi(x_i) = \exp(-x_i^2)\left[1 \quad \sqrt{\tfrac{2}{1!}}x_i \quad \sqrt{\tfrac{2^2}{2!}}x_i^2 \quad \sqrt{\tfrac{2^3}{3!}}x_i^3 \quad \cdots\right].$$

Kernel Trick for Structured Data

- Kernel trick is useful for structured data:
  - Consider data that doesn't look like this:

$$X = \begin{bmatrix} 0.5377 & 0.3188 & 3.5784 \\ 1.8339 & -1.3077 & 2.7694 \\ -2.2588 & -0.4336 & -1.3499 \\ 0.8622 & 0.3426 & 3.0349 \end{bmatrix}, \quad y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix},$$

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  - We could convert sentences to features, or define kernel between sentences.
  - For example, "string" kernels:
    - Weighted frequency of common subsequences (dynamic programming).
  - There are also "graph kernels", "image kernels", and so on...

Valid Kernels

- What kernel functions $k(x_i, x_j)$ can we use?
- Kernel k must be an inner product in some space:
  - There exists ϕ such that $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$.

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We can decompose a (continuous or finite-domain) function k into

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  - Show explicitly that $k(x_i, x_j)$ is an inner product.
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- Nice in theory, what do we do in practice?
  - Show explicitly that $k(x_i, x_j)$ is an inner product.
  - Or show it can be constructed from other valid kernels.
- If we use invalid kernel, lose inner-product interpretation but may work fine.

Bonus Slide: Constructing Feature Space

- Why is positive semi-definiteness important?
  - With finite domain we can define K over all points.
  - The condition $K \succeq 0$ means it has a spectral decomposition

$$K = U^T \Lambda U,$$

    where the eignevalues $\lambda_i \geq 0$ and so we have a real $\Lambda^{\frac{1}{2}}$.
  - Thus we hav $K = U^T \Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} U = \|\Lambda^{\frac{1}{2}} U\|^2$ and we could use

$$\Phi(X) = \Lambda^{\frac{1}{2}} U, \text{ or } \phi(x_i) = \Lambda^{\frac{1}{2}} U_{:,i}.$$

- The above reasoning isn't quite right for continuous domains.
- The more careful generalization is known as "Mercer's theorem".

Constructing Valid Kernels

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  - $\exp(k_1(x_i, x_j))$.

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  - $k_1(x_i, x_j) k_2(x_i, x_j)$.
  - $\phi(x_i) k_1(x_i, x_j) \phi(x_j)$.
  - $\exp(k_1(x_i, x_j))$.
- Example: Gaussian-RBF kernel:

$$
\begin{aligned}
k(x_i, x_j) &= \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right) \\
&= \underbrace{\exp\left(-\frac{\|x_i\|^2}{\sigma^2}\right)}_{\phi(x_i)} \underbrace{\exp\left(\underbrace{\frac{2}{\sigma^2}}_{\alpha \geq 0} \underbrace{x_i^T x_j}_{\text{valid}}\right)}_{\exp(\text{valid})} \underbrace{\exp\left(-\frac{\|x_j\|^2}{\sigma^2}\right)}_{\phi(x_j)}.
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    - k-nearest neighbours.
    - Clustering algorithms (k-means, density-based clustering, hierarchical clustering).
    - Amazon item-to-item product recommendation.
    - Non-parametric regression.
    - Outlier ratio.
    - Multi-dimensional scaling.
    - Graph-based semi-supervised learning.

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- Besides ridge regression, when can we apply the kernel trick?
  - Distance-based methods (see my undergrad course):

$$\|x_i - x_j\|^2 = \langle x_i, x_j \rangle - 2\langle x_i, x_j \rangle + \langle x_j, x_j \rangle.$$

    - k-nearest neighbours.
    - Clustering algorithms (k-means, density-based clustering, hierarchical clustering).
    - Amazon item-to-item product recommendation.
    - Non-parametric regression.
    - Outlier ratio.
    - Multi-dimensional scaling.
    - Graph-based semi-supervised learning.
  - Eigenvalue methods:
    - Principle component analysis (trick for centering in high-dimensional space).
    - Canonical correlation analysis.
    - Spectral clustering.
  - L2-regularized linear models...

Representer Theorem

- Consider linear model differentiable with losses f_i and L2-regularization,

$$\operatorname*{argmin}_{w \in \mathbb{R}^d} \sum_{i=1}^{n} f_i(w^T x_i) + \frac{\lambda}{2}\|w\|^2.$$

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- So any solution w^* can written as a linear combination of features x_i,

$$\begin{aligned} w^* &= -\frac{1}{\lambda} \sum_{i=1}^{n} f_i'((w^*)^T x_i) x_i = \sum_{i=1}^{n} z_i x_i \\ &= X^T z. \end{aligned}$$

- This is called a representer theorem (true under much more general conditions).

Representer Theorem

- Using representer theorem we can use $w = X^T z$ in original problem,

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- Now defining $f(z) = \sum_{i=1}^{n} f_i(z_i)$ for a vector z we have

$$\begin{aligned}
&= \operatorname*{argmin}_{z \in \mathbb{R}^n} f(XX^T z) + \frac{\lambda}{2} z^T XX^T z \\
&= \operatorname*{argmin}_{z \in \mathbb{R}^n} f(Kz) + \frac{\lambda}{2} z^T K z.
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- Similarly, at test time we can use the n variables z,

$$\hat{X}w = \hat{X}X^T z = \hat{K}z.$$

(pause)

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- For convex f and g and the primal problem

$$\operatorname*{argmin}_{w \in \mathbb{R}^d} P(w) = f(Xw) + g(w),$$

the Fenchel dual is given by

$$\operatorname*{argmax}_{z \in \mathbb{R}^n} D(z) = -f^*(-z) - g^*(X^T z),$$

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  - Dual sometimes allows sparse kernel representation.

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- Generalization of max that includes limits:

$$\max_{x \in \mathbb{R}} -x^2 = 0, \quad \sup_{x \in \mathbb{R}} -x^2 = 0,$$

but

$$\max_{x \in \mathbb{R}} -e^x = \text{DNE}, \quad \sup_{x \in \mathbb{R}} -e^x = 0.$$

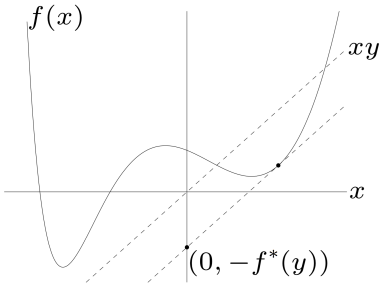
- The analogy for min is called the infimum.

Convex Conjugate

- The convex conjugate f^* of a function f is given by

$$f^*(y) = \sup_{x \in \mathcal{D}} \{y^T x - f(x)\},$$

where $\mathcal{D}$ is values where $\sup$ is finite.



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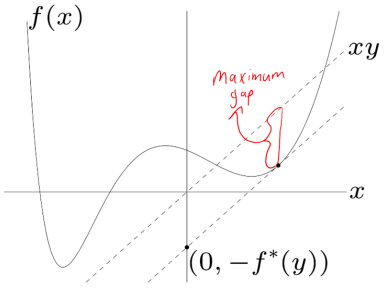

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- It's the maximum that the linear function $y^T x$ can get above $f(x)$.

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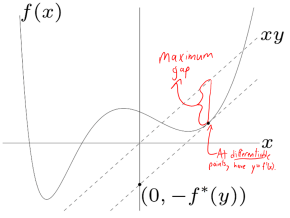

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- If f is differentable, then $\sup$ occurs at x where $y = \nabla f(x)$.
- Note that f^* is convex even if f is not.
- If f is convex (and "closed"), then $f^{**} = f$.

Convex Conjugate Examples

- If $f(x) = \frac{1}{2}\|x\|^2$ we have
  - $f^*(y) = \sup_x\{y^T x - \frac{1}{2}\|x\|^2\}$ or equivalently (by taking derivative and setting to 0):

$$0 = y - x,$$

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$$f^*(y) = \sup_x\{y^T x - a^T x\} = \sup_x\{(y-a)^T x\} = \begin{cases} 0 & y = a \\ \infty & \text{otherwise.} \end{cases}$$

- For other examples, see Boyd & Vandenberghe.

Fenchel Dual of SVMs

- Consider support vector machines,

$$\underset{w\in\mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2}\|w\|^2.$$

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  - Case where coordinate optimization is efficient.

Stochastic Dual Coordinate Ascent

- If we have an L2-regularized linear model with convex f_i,

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then the Fenchel dual is given by

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- We can apply stochastic dual coordinate ascent (SDCA):
  - Only looks at one training example on each iteration.
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    - Performance similar to SAG for many problems, worse if $\mu >> \lambda$.

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  - Obtains $O(1/\epsilon)$ rate for non-smooth f:
    - Same rate as stochastic subgradient, but we can now use exact/adaptive step-size.
    - You could add an L2-regularizer to dual, corresponds to smoothing primal.

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- Valid kernels are typically constructed from other valid kernels.
- Representer theorem allows kernel trick for L2-regularized linear models.
- Fenchel dual re-writes sum of convex functions with convex conjugates:
  - Dual may have nice structure: differentiable, sparse, coordinate optimization.

- Final session: we discuss parrallel/distributed methods and non-convex functions.