CPSC 540: Machine Learning MAP Estimation, Convex Functions

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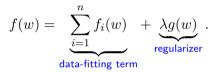
Admin

• Auditting/registration forms:

- Submit them at end of class, pick them up end of next class.
- I need your prereq form before I'll sign registration forms.
- Website/Piazza:
 - https://www.cs.ubc.ca/~schmidtm/Courses/540-W17.
 - https://piazza.com/ubc.ca/winterterm22016/cpsc540.
- Tutorials: start this Friday (4:00 in DMP 110).
- Assignment 1 due January 16.
 - 1 late day to hand it in January 18.
 - 2 late days to hand it in January 23.

Last Time: Loss Plus Regularizer Framework

• We discussed the typical "minimizing loss plus regularizer" framework,



- Loss function f_i measures how well we fit example i with parameters w.
- Regularizer g measures how complicated the model is with parameters w.
- Regularization parameter $\lambda > 0$ controls strength of regularization:
 - Usually set by using a validation set or with cross-validation.

Last Time: L2-Regularized Least Squares

• One of the simplest examples is L2-regularized least squares:

$$f(w) = \frac{1}{2} \sum_{i=1}^{n} (w^{T} x^{i} - y^{i})^{2} + \frac{\lambda}{2} \sum_{j=1}^{d} w_{j}^{2},$$

• We showed how to write this in matrix and norm notation:

$$f(w) = \frac{1}{2} \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|^2.$$

• We showed how to derive the gradient and minimum of quadratics,

$$\nabla f(w) = X^T X w - X^T y + \lambda w, \quad w^* = (X^T X + \lambda I)^{-1} (X^T y).$$

• We showed how to derive the Hessian and that it is positive-definite,

$$\nabla^2 f(w) = X^T X + \lambda I \succ 0.$$

• Today: a probabilistic perspective on the loss plus regularizer framework.

Logistic Regression for Binary y^i

• After squared error, second most common loss function is logistic loss,

$$f(w) = \sum_{i=1}^{n} \log(1 + \exp(-y^{i}w^{T}x^{i})) + \frac{\lambda}{2} \|w\|^{2},$$

for binary $y^i \in \{-1, +1\}$ and where we make predictions using $\hat{y}^i = \operatorname{sign}(w^T \hat{x}^i)$. • This is not a norm, so where does it come from?

- When $\lambda = 0$, this is derived as a maximum likelihood estimate (MLE).
- When $\lambda > 0$, this is derived as a maximum a posteriori (MAP) estimate.

Maximum Likelihood Estimation (MLE)

- MLE in an abstract setting:
 - We have a dataset *D*.
 - We want to pick a model h among a set of models \mathcal{H} .
 - We define the likelihood as the probability mass/density function p(D|h).
 - We choose the model h^* that maximizes the likelihood,

 $h^* \in \operatorname*{argmax}_{h \in \mathcal{H}} p(D|h).$

- MLE has appealing "consistency" properties as $n \to \infty$ (take STAT 560/561).
- In the case of regression, we usually maximize the conditional likelihood,

p(y|X, w),

where we condition on the features X.

Minimizing the Negative Log-Likelihood

• To maximize the likelihood, usually we minimize the negative log-likelihood,

$$h^* \in \mathop{\mathrm{argmax}}_{h \in \mathcal{H}} p(D|h) \equiv \mathop{\mathrm{argmin}}_{h \in \mathcal{H}} - \log p(D|h),$$

- This yields same solution.
 - Logarithm is monotonic: if $\alpha > \beta$ then $\log(\alpha) > \log(\beta)$.
 - Changing sign flips max to min.
- See "Max and Argmax" notes on the webpage if the above seems strange.

Minimizing the Negative Log-Likelihood

• We use logarithm because it turns multiplication into addition,

 $\log(\alpha\beta) = \log(\alpha) + \log(\beta),$

or more generally

$$\log\left(\prod_{i=1}^{n} a_i\right) = \sum_{i=1}^{n} \log(a_i).$$

• If data is n IID samples D_i then $p(D|h) = \prod_{i=1}^n p(D_i|h),$ and our MLE is

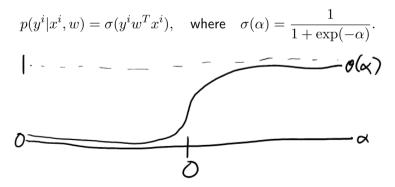
$$h^* \in \operatorname*{argmax}_{h \in \mathcal{H}} \prod_{i=1}^n p(D_i|h) \equiv \operatorname*{argmin}_{h \in \mathcal{H}} - \sum_{i=1}^n \log p(D_i|h).$$

MLE Interpretation of Logistic Regression

• For IID regression problems the conditional negative log-likelihood can be written

$$-\log p(y|X,w) = -\log \left(\prod_{i=1}^{n} p(y^{i}|x^{i},w)\right) = -\sum_{i=1}^{n} \log p(y^{i}|x^{i},w).$$

• Logistic regression assumes conditional likelihood using sigmoid function σ ,



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• Logistic regression assumes conditional likelihood using sigmoid function σ ,

$$p(y^i|x^i,w) = \sigma(y^iw^Tx^i), \quad \text{where} \quad \sigma(\alpha) = rac{1}{1+\exp(-\alpha)}.$$

• Plugging in the sigmoid we get

$$f(w) = -\sum_{i=1}^n \log\left(\frac{1}{1 + \exp(-y^i w^T x^i)}\right) = \sum_{i=1}^n \underbrace{\log(1 + \exp(-y^i w^T x^i))}_{\text{logistic loss}},$$

using $\log(1) = 0$.

• Many loss functions are equivalent to negative log-likelihoods.

Least Squares as Conditional-Gaussian MLE

• Recall the Gaussian (normal) distribution,

$$p(\alpha|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(\mu-\alpha)^2}{2\sigma^2}\right).$$

• Least squares is MLE assuming Gaussian conditional likelihood with mean $w^T x^i$,

$$\begin{split} p(y^i|x^i, w, \sigma^2) &= \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(w^T x^i - y^i)^2}{2\sigma^2}\right) \\ &\propto \exp\left(-\frac{(w^T x^i - y^i)^2}{2\sigma^2}\right), \end{split}$$

where for probabilities \propto means "equal up to a constant not depending on $y^{i^{\prime\prime}}.$

• Another way we'll write this assumption is

$$y^i \sim \mathcal{N}(w^T x^i, \sigma^2),$$

which is read " y^i is generated from a Gaussian with mean $w^T x^i$ and variance $\sigma^{2"}$.

Least Squares as Conditional-Gaussian MLE

• Least squares is the MLE under our assumption that $y^i \sim \mathcal{N}(w^T x^i, \sigma^2)$,

$$\begin{split} w^* &\in \operatorname*{argmin}_{w \in \mathbb{R}^d} \sum_{i=1}^n -\log p(y^i | w, x^i) \\ &\equiv \operatorname*{argmin}_{w \in \mathbb{R}^d} \sum_{i=1}^n -\log \left(\frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{(w^T x^i - y^i)^2}{2\sigma^2} \right) \right) \\ &\equiv \operatorname*{argmin}_{w \in \mathbb{R}^d} \sum_{i=1}^n \left[-\log \left(\frac{1}{\sigma \sqrt{2\pi}} \right) + \frac{(w^T x^i - y^i)^2}{2\sigma^2} \right]. \end{split}$$

• Notice that constant doesn't depend on w so doesn't change argmin,

$$\equiv \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \frac{1}{2\sigma^2} \sum_{i=1}^n (w^T x^i - y^i)^2 \equiv \underbrace{\underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \frac{1}{2} \sum_{i=1}^n (w^T x^i - y^i)^2}_{\text{least squares}},$$

where we note that $\sigma > 0$ doesn't change argmin.

Maximum Likelihood Estimation and Overfitting

• In our abstract setting with data D the MLE is

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h^* \in \operatorname*{argmax}_{h \in \mathcal{H}} p(D|h).
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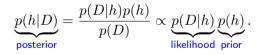
- But conceptually MLE is a bit weird:
 - "Find the h that makes D have the highest probability given h".
- And MLE often leads to overfitting:
 - Data could be very likely in some very unlikely model from family.
 - For example, a complex model overfits by memorizing the data.
- What we really want:
 - "Find the h that is the most likely given the data D"'.

Maximum a Posteriori (MAP) Estimation

• Maximum a posteriori (MAP) estimate maximizes the reverse probability,

```
h^* \in \operatorname*{argmax}_{h \in \mathcal{H}} p(h|D).
```

- This is what we want: the probability of h given our data.
- MLE and MAP are connected by Bayes' rule,



- So MAP maximizes the likelihood p(D|h) times the prior p(h):
 - $\bullet\,$ Prior is our "belief" that h is correct model before seeing data.
 - Prior can reflect that complex models are likely to overfit.

MAP Estimation and Regularization

• From Bayes rule the MAP estimate with IID examples D_i is

$$h^* \in \operatorname*{argmax}_{h \in \mathcal{H}} p(h|D) \equiv \operatorname*{argmax}_{h \in \mathcal{H}} \prod_{i=1}^n \left[p(D|h) \right] p(h).$$

• By again taking the negative logarithm we get

$$h^* \in \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{n} \underbrace{-\log p(D_i|h)}_{\operatorname{loss}} - \underbrace{\log p(h)}_{\operatorname{regularizer}},$$

so we can view the negative log-prior as a regularizer.

• Many regularizers are equivalent to negative log-priors.

L2-Regularization and MAP Estimation

 ${\ensuremath{\, \bullet }}$ We obtain L2-regularization under an independent Gaussian assumption,

 $w_j \sim \mathcal{N}(0, 1/\lambda).$

• This implies that

$$p(w) = \prod_{j=1}^{d} p(w_j|\lambda) \propto \prod_{j=1}^{d} \exp\left(-\frac{\lambda}{2}w_j^2\right) = \exp\left(-\frac{\lambda}{2}\sum_{j=1}^{d}w_j^2\right).$$

so we have that

$$-\log p(w) = -\log \exp\left(-\frac{\lambda}{2}||w||^2\right) = \frac{\lambda}{2}||w||^2.$$

• So the MAP estimate with IID training examples would be

$$w^* \in \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} - \log p(y|X, w) - \log p(w) \equiv \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^n - \log p(y^i|x^i, w) + \frac{\lambda}{2} \|w\|^2.$$

MAP Estimation Perspective

- Many of our loss functions and regularizers have probabilistic interpretations.
 - For example, Laplace likelihood leads to absolute error and L1-regularization.
- Probabilitic interpretation lets us define regression losses in non-standard settings:
 - Multi-label y^i .
 - Multi-class y^i .
 - Ordinal y^i .
 - Count y^i .
 - Survival time y^i .

Outline

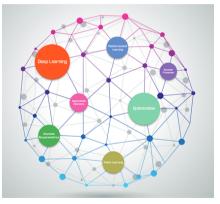
1 MAP Estimation

2 Minimizing Maxes of Linear Functions

3 Convex Functions

Current Hot Topics in Machine Learning

• Graph of most common keywords among ICML papers in 2015:



• Why is there so much focus on deep learning and optimization?

Why Study Optimization in CPSC 540?

• In machine learning, training is typically written as optimization:

- Numerically optimize parameters w of model, given data.
- There are some exceptions:
 - Ounting- and distance-based methods (KNN, random forests).
 - See CPSC 340.
 - Integration-based methods (Bayesian learning).
 - Later in course.

Although you still need to tune parameters in those models.

- But why study optimization? Can't I just use optimization libraries?
 - "\", linprog, quadprog, fminunc, fmincon, CVX, and so.

The Effect of Big Data and Big Models

- Datasets are getting huge, we might want to train on:
 - Entire medical image databases.
 - Every webpage on the internet.
 - Every product on Amazon.
 - Every rating on Netflix.
 - All flight data in history.
- With bigger datasets, we can build bigger models:
 - Complicated models can address complicated problems.
 - Regularized linear models on huge datasets are standard industry tool.
 - Deep learning allows us to learn features from huge datasets.
- But optimization becomes a bottleneck because of time/memory.
 - ${\ensuremath{\, \circ }}$ We can't afford $O(d^2)$ memory, or an $O(d^2)$ operation.
 - Going through huge datasets hundreds of times is too slow.
 - Evaluating huge models many times may be too slow.
- Next class we'll start large-scale machine learning.
 - But first we'll show how to use some "off the shelf" optimization methods.

Robust Regression in Matrix Notation

• Regression with the absolute error as the loss,

$$f(w) = \sum_{i=1}^{n} |w^T x^i - y^i|.$$

- In CPSC 340 we argued that this is more robust to outliers.
- We can write this in matrix notation as

$$f(w) = \|Xw - y\|_1.$$

where recall that the L1-norm of a vector r of length n is

$$|r||_1 = \sum_{i=1}^n |r_i|.$$

- This objective is not quadratic, but can be minimized as a linear program.
 - Minimizing a linear function with linear constraints.

Robust Regression as a Linear Program

• L1-norm regression in summation notation,

$$\underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^n |w^T x^i - y^i|.$$

• Re-write absolute value using $|\alpha|=\max\{\alpha,-\alpha\}$,

$$\underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^n \max\{w^T x^i - y^i, y^i - w^T x^i\}.$$

• Introduce n variables r_i that upper bound the max functions,

$$\underset{w \in \mathbb{R}^{d}, r \in \mathbb{R}^{n}}{\operatorname{argmin}} \sum_{i=1}^{n} r_{i}, \quad \text{with} \quad r_{i} \geq \max\{w^{T} x^{i} - y^{i}, y^{i} - w^{T} x^{i}\}, \forall i.$$

- This is a linear objective with non-linear constraints.
- Note that we have $r_i = |w^T x^i y^i|$ at the solution.
 - Otherwise, either the constraints are violated or we could decrese r_i .

Robust Regression as a Linear Program

• L1-norm regression in summation notation,

1

$$\underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^n |w^T x^i - y^i|.$$

• Re-write absolute value using $|\alpha|=\max\{\alpha,-\alpha\}$,

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• Introduce n variables r_i that upper bound the max functions,

$$\underset{v \in \mathbb{R}^{d}, r \in \mathbb{R}^{n}}{\operatorname{argmin}} \sum_{i=1}^{n} r_{i}, \quad \text{with} \quad r_{i} \geq \max\{w^{T} x^{i} - y^{i}, y^{i} - w^{T} x^{i}\}, \forall i.$$

• Having r_i bound the max is equivalent to r_i bounding max arguments.

$$\underset{w \in \mathbb{R}^{d}, r \in \mathbb{R}^{n}}{\operatorname{argmin}} \sum_{i=1}^{n} r_{i}, \quad \text{with} \quad r_{i} \geq w^{T} x^{i} - y^{i}, \; r_{i} \geq y^{i} - w^{T} x^{i}, \forall i.$$

Robust Regression as a Linear Program

• We've shown that L1-norm regression can be written as a linear program,

$$\underset{w \in \mathbb{R}^{d}, r \in \mathbb{R}^{n}}{\operatorname{argmin}} \sum_{i=1}^{n} r_{i}, \quad \text{with} \quad r_{i} \geq w^{T} x^{i} - y^{i}, \; r_{i} \geq y^{i} - w^{T} x^{i}, \forall i,$$

or in matrix notation as

$$\underset{w \in \mathbb{R}^d, \ r \in \mathbb{R}^n}{\operatorname{argmin}} \ \mathbf{1}^T r, \quad \text{with} \quad r \ge Xw - y, \ r \ge y - Xw,$$

where 1 is a vector containing all ones and inequalities are element-wise.

• For medium-sized problems, we can solve this with Matlab's *linprog*.

Minimizing Absolute Values and Maxes

- A general approach for minimizing absolute values and/or maximums:
 - **1** Introduce maximums over linear functions to replace minimizing absolute values.
 - Introduce new variables that are constrained to bound the maximums.
 - **③** Transform to linear constraints by splitting the maximum constraints.
- For example, we can write minimizing support vector machine (SVM) objective,

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y^{i} w^{T} x^{i}\} + \frac{\lambda}{2} \|w\|^{2},$$

as a quadratic program (quadratic objective with linear constraints).

Support Vector Machine as a Quadratic Program

• The SVM optimization problem is

$$\underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^n \max\{0, 1 - y^i w^T x^i\} + \frac{\lambda}{2} \|w\|^2,$$

Introduce new variables to upper-bound the maxes,

$$\underset{w \in \mathbb{R}^{d}, r \in \mathbb{R}^{n}}{\operatorname{argmin}} \sum_{i=1}^{n} r_{i} + \frac{\lambda}{2} \|w\|^{2}, \quad \text{with} \quad r \geq \max\{0, 1 - y^{i}w^{T}x^{i}\}, \forall i.$$

• Split the maxes into separate constraints,

$$\underset{w \in \mathbb{R}^d, r \in \mathbb{R}^n}{\operatorname{argmin}} \ 1^T r + \frac{\lambda}{2} \|w\|^2, \quad \text{with} \quad r \geq 0, \ r \geq YXw,$$

where Y is a diagonal matrix with the y^i values along the diagonal.

• This means YX is X with each row scaled by the corresponding y^i .



1 MAP Estimation

2 Minimizing Maxes of Linear Functions



General Lp-norm Losses

• Consider minimizing the regression loss

$$f(w) = \|Xw - y\|_p,$$

where $\|\cdot\|_p$ is a general Lp-norm,

$$||r||_p = \left(\sum_{i=1}^n |r_i|^p\right)^{\frac{1}{p}}$$

.

• Recall the three properties of norms:

 $\|r+u\| \le \|r\| + \|u\|,$

and that these imply norms are non-negative.

(absolute homogeneity) (triangle inequality)

General Lp-norm Losses

• Consider minimizing the regression loss

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where $\|\cdot\|_p$ is a general Lp-norm,

$$\|r\|_p = \left(\sum_{i=1}^n |r_i|^p\right)^{\frac{1}{p}}$$

- With p = 2, we can minimize the function using linear algebra.
 - By non-negativity, squaring it doesn't change the argmax.
- With p = 1, we can minimize the function using linear programming.
- With $p = \infty$, we can also use linear programming.
- For 1 , we can use gradient descent (next lecture).
 - It's smooth once raise to the power p.

• If we use p < 1 (which is not a norm), minimizing f is NP-hard.

- With $p \ge 1$ the problem is convex, while with p < 1 the problem is non-convex.
- Convexity is usually a good indicator of tractability:
 - Minimizing convex functions is usually easy.
 - Minimizing non-convex functions is usually hard.
- Existing software (like CVX) minimizes a wide variety of convex functions.
- To define convex functions, we first need the notion of a convex combination:
 - ${\ensuremath{\, \bullet }}$ A convex combination of two variables w and v is given by

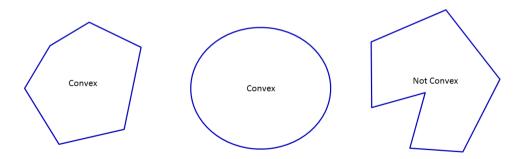
$$\theta w + (1-\theta) v \quad \text{for any} \quad 0 \leq \theta \leq 1.$$

• A convex combination of k variables $\{w_1, w_2, \ldots, w_k\}$ is given by

$$\sum_{c=1}^k \theta_c w_c \quad \text{where} \quad \sum_{c=1}^k \theta_c = 1, \; \theta_c \geq 0.$$

Convex Sets

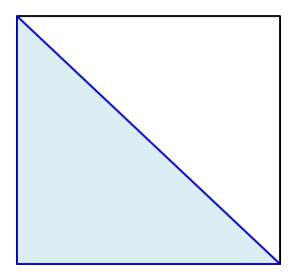
- The domain of a convex function must be a convex set:
 - \bullet A set ${\mathcal C}$ is convex if convex combinations of points in the set are also in the set.
 - For all $w \in C$ and $v \in C$ we have $\theta w + (1 \theta)v \in C$ for $0 \le \theta \le 1$.



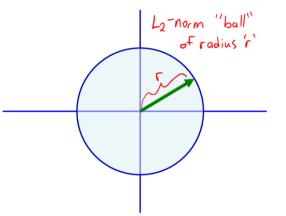
- Real space \mathbb{R}^d .
- Positive orthant $\mathbb{R}^d_+ : \{ w \mid w \ge 0 \}.$
- Hyper-plane: $\{w \mid a^T w = b\}.$
- Half-space: $\{w \mid a^T w \leq b\}.$
- Norm-ball: $\{w \mid ||w||_p \leq \tau\}.$
- Norm-cone $\{(w, \tau) \mid ||w||_p \le \tau\}.$

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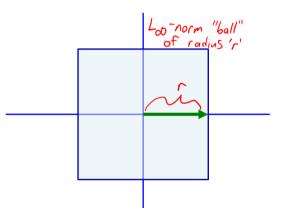


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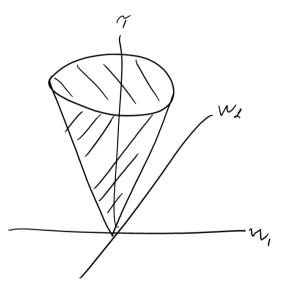
Examples of Simple Convex Sets

- Real space \mathbb{R}^d .
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Showing a Set is Convex from Defintion

- We can prove convexity of a set from the definition:
 - Choose a generic w and v in C, show that generic u between them is in the set.
- Hyper-plane example: $C = \{w \mid a^T w = b\}.$
 - If $w \in \mathcal{C}$ and $v \in \mathcal{C}$, then we have $a^T w = b$ and $a^T v = b$.
 - To show C is convex, we can show that $a^T u = b$ for u between w and v.

$$a^{T}u = a^{T}(\theta w + (1 - \theta)v)$$
$$= \theta(a^{T}w) + (1 - \theta)(a^{T}v)$$
$$= \theta b + (1 - \theta)b = b.$$

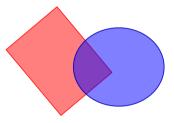
Showing a Set is Convex from Defintion

- We can prove convexity of a set from the definition:
 - Choose a generic w and v in \mathcal{C} , show that generic u between them is in the set.
- Norm-ball example: $C = \{w \mid ||w||_p \le 10\}.$
 - If $w \in \mathcal{C}$ and $v \in \mathcal{C}$, then we have $\|w\|_p \leq 10$ and $\|v\|_p \leq 10$.
 - To show C is convex, we can show that $||u||_p \leq 10$ for u between w and v.

$$\begin{split} \|u\|_{p} &= \|\theta w + (1-\theta)v\|_{p} \\ &\leq \|\theta w\|_{p} + \|(1-\theta)v\|_{p} \qquad \text{(triangle inequality)} \\ &= |\theta| \cdot \|w\|_{p} + |1-\theta| \cdot \|v\|_{p} \qquad \text{(absolute homogeneity)} \\ &= \theta \|w\|_{p} + (1-\theta)\|v\|_{p} \qquad (0 \leq \theta \leq 1) \\ &\leq \theta 10 + (1-\theta) 10 = 10. \end{split}$$

Showing a Set is Convex from Intersections

- The intersection of convex sets is convex.
 - Proof is trivial: convex combinations in the intersection are in the intersection.



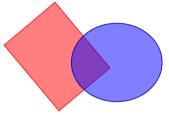
• We can prove convexity of a set by showing it's an intersection of convex sets.

• Example:
$$\{w|a^Tw = b, \|w\|_p \le 10\}$$
 is convex.

• It's the intersection of our two previous examples.

Showing a Set is Convex from Intersections

- The intersection of convex sets is convex.
 - Proof is trivial: convex combinations in the intersection are in the intersection.

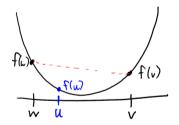


- We can prove convexity of a set but showing it's an intersection of convex sets.
- Example: the w satisfying linear constraints form a convex set:

$$\begin{aligned} Aw &\leq b \\ A_{eq}w &= b_{eq} \\ LB &\leq w \leq UB. \end{aligned}$$

- Two equivalent definitons of aconvex function:
 - Area above the function is a convex set.
 - ② The function is always below the "chord" between two points.

$$f(\theta w + (1-\theta)v) \le \theta f(w) + (1-\theta)f(v), \quad \text{for all } w \in \mathcal{C}, v \in \mathcal{C}, 0 \le \theta \le 1.$$



- Implications: all local minima are global minima.
- We can globally minimize a convex function by finding any stationary point.

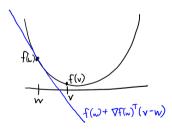
Examples of Convex Functions

- 1D quadratic: $aw^2 + bw + c$, when a > 0.
- Linear: $a^T w + b$.
- Exponential: $\exp(aw)$.
- Negative logarithm: $-\log(w)$.
- Absolute value: |w|.
- Max: $\max_i \{w_i\}$.
- Negative entropy: $w \log w$, for w > 0.
- Logistic loss: $\log(1 + \exp(-w))$.
- Log-sum-exp: $\log(\sum_i \exp(w))$.

Differentiable Convex Functions

- Convex functions must be continuous, and have a domain that is a convex set.
 - But they may be non-differentiable.
- For differentiable convex functions, there is third equivalent definiton:
 - A differentiable f is convex iff f is always above tangent.

$$f(v) \ge f(w) + \nabla f(w)^T (v - w), \quad \forall w \in \mathcal{C}, v \in \mathcal{C}.$$



• Notice that $\nabla f(w) = 0$ implies $f(v) \ge f(w)$ for all v, so w is a global minimizer.

Twice-Differentiable Convex Functions

- For twice-differentiable convex functions, there is a fourth equivalent definition:
 - A *twice-differentiable* f is convex iff f is curved upwards everywhere.
- For univariate functions, this means $f''(w) \ge 0$ for all w.
 - Usually the easiest way to show a twice-differentiable f is convex.
- For multivariate functions, means the Hessian is positive semi-definite for all w,

$$\nabla^2 f(w) \succeq 0,$$

meaning that $v^T \nabla^2 f(w) v \ge 0$ for all w and v.

Convexity and Least Squares

• We can use twice-differentiable definition to show convexity of least squares,

$$f(w) = \frac{1}{2} \|Xw - y\|^2.$$

• Using results from last time we have

$$\nabla^2 f(w) = X^T X = \sum_{i=1}^n x^i (x^i)^T$$

- So we want to show that $X^T X \succeq 0$ or equivalently that $v^T X^T X v \ge 0$ for all v.
- We did this last time in matrix notation, let's do it in summation notation:

$$v^T \left(\sum_{i=1}^n x^i (x^i)^T \right) v = \sum_{i=1}^n v^T x_i (x_i)^T v = \sum_{i=1}^n (v^T x_i) \left((x_i)^T v \right) = \sum_{i=1}^n (v^T x^i)^2 \ge 0,$$

so least squares is convex and setting $\nabla f(w) = 0$ gives global minimum.

Operations that Preserve Convexity

- There are a few operations that preserve convexity.
 - Can show convexity by writing as sequence of convexity-preserving operations.
- If f and g are convex functions, the following preserve convexity:
 Non-negative scaling: h(w) = α f(w).
 - 2 Sum: h(w) = f(w) + g(w).
 - Solution Maximum: $h(w) = \max\{f(w), g(w)\}.$
 - Omposition with affine map:

$$h(w) = f(Aw + b),$$

where an affine map $w \mapsto Aw + b$ is a multi-input multi-output linear function.

• But note that composition f(g(w)) is not convex in general.

Convexity of SVMs

- If f and g are convex functions, the following preserve convexity:
 - Non-negative scaling.
 - 2 Sum.
 - Maximum.
 - Omposition with affine map.
- We can use these to quickly show that SVMs are convex,

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y^{i}w^{T}x^{i}\} + \frac{\lambda}{2} \|w\|^{2}.$$

- Second term has a Hessian of λI so is convex because $\lambda I \succeq 0$.
- First term is sum(max(linear)). Linear is convex and sum/max preserve convexity.
- Since both terms are convex, and sums preserve convexity, SVMs are convex.

Summary

- MLE and MAP estimation give probabilistic interpretation to losses/regularizers.
- Converting non-smooth problems involving max to constrained smooth problems.
- Convex functions are special functions where all stationary points are global minima.
- Showing functions are convex from definitions or convexity-preserving operations.
- How do we solve "large-scale" problems?

Bonus Slide: \propto Probability Notation

• When we write

 $p(y) \propto f(y),$

we mean that

$$p(y) = \kappa f(y),$$

where κ is the number need to make p a probability.

• If y is discrete taking values in \mathcal{Y} ,

$$\kappa = \frac{1}{\sum_{y \in \mathcal{Y}} f(y)}.$$

• If y is continuous taking values in \mathcal{Y} ,

$$\kappa = \frac{1}{\int_{y \in \mathcal{Y}} f(y)}.$$

• Return to Gaussian MLE.