



Convex Optimization

DS-GA 1013 / MATH-GA 2824 Mathematical Tools for Data Science

https://cims.nyu.edu/~cfgranda/pages/MTDS_spring19/index.html

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Motivating applications

Convex functions

Optimality conditions

Convex Regularization

Optimization algorithms

Sparse regression

Linear regression is challenging when the number of features p is large

Problem: How to choose subset of features $\mathcal{I} \subset \{1, \dots, p\}$, such that

$$y \approx \sum_{i \in \mathcal{I}} \vec{\beta}[i] \vec{x}[i] + \beta_0$$

Equivalently, find sparse coefficient vector $\vec{\beta} \in \mathbb{R}^p$ such that

$$y \approx \langle \vec{x}, \vec{\beta} \rangle + \beta_0$$

Collaborative filtering

Quantity $y[i, j]$ depends on indices i and j

We observe examples and want to predict new instances

For example, $y[i, j]$ is rating given to a movie i by a user j

Collaborative filtering

							...
	★★★★★	?	★★★★☆	?	?	?	...
	?	★★★★☆	?	?	★★★★☆	?	...
	?	?	?	★★★★☆	★★★★☆	?	...
	?	★★★★☆	★★★★☆	?	?	★★★★★	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Rank- r bilinear model

Certain people like certain movies: r factors

$$y[i, j] \approx \sum_{l=1}^r a_l[i] b_l[j]$$

For each factor l

- ▶ $a_l[i]$: movie i is positively (> 0), negatively (< 0) or not (≈ 0) associated to factor l
- ▶ $b_l[j]$: user j is positively (> 0), negatively (< 0) or not (≈ 0) associated to factor l

SVD can be used to fit the model if **all** entries are observed

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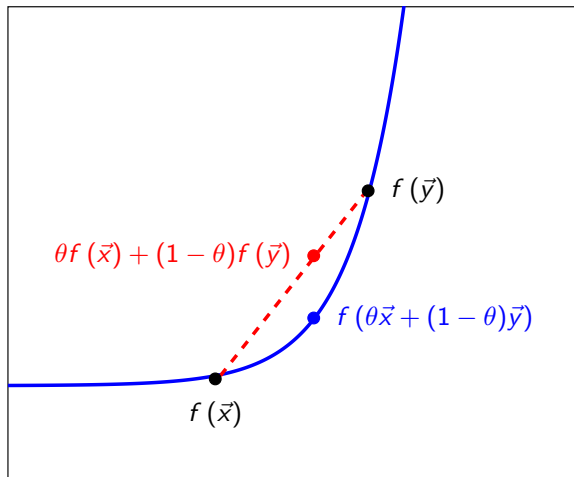
Optimization algorithms

Convex functions

A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is **convex** if for any $\vec{x}, \vec{y} \in \mathbb{R}^n$ and any $\theta \in (0, 1)$

$$\theta f(\vec{x}) + (1 - \theta) f(\vec{y}) \geq f(\theta \vec{x} + (1 - \theta) \vec{y})$$

Convex functions



Linear functions are convex

If f is linear

$$f(\theta \vec{x} + (1 - \theta) \vec{y})$$

Linear functions are convex

If f is linear

$$f(\theta \vec{x} + (1 - \theta) \vec{y}) = \theta f(\vec{x}) + (1 - \theta) f(\vec{y})$$

Strictly convex functions

A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is **strictly** convex if for any $\vec{x}, \vec{y} \in \mathbb{R}^n$ and any $\theta \in (0, 1)$

$$\theta f(\vec{x}) + (1 - \theta) f(\vec{y}) > f(\theta \vec{x} + (1 - \theta) \vec{y})$$

Local minima are global

Any local minimum of a convex function is also a global minimum

Proof

Let $\vec{x}_{\text{loc}}$ be a local minimum: for all $\vec{x} \in \mathbb{R}^n$ such that $\|\vec{x} - \vec{x}_{\text{loc}}\|_2 \leq \gamma$

$$f(\vec{x}_{\text{loc}}) \leq f(\vec{x})$$

Let $\vec{x}_{\text{glob}}$ be a global minimum

$$f(\vec{x}_{\text{glob}}) < f(\vec{x}_{\text{loc}})$$

Proof

Choose θ so that $\vec{x}_\theta := \theta \vec{x}_{\text{loc}} + (1 - \theta) \vec{x}_{\text{glob}}$ satisfies

$$\|\vec{x}_\theta - \vec{x}_{\text{loc}}\|_2 \leq \gamma$$

then

$$f(\vec{x}_{\text{loc}}) \leq f(\vec{x}_\theta)$$

Proof

Choose θ so that $\vec{x}_\theta := \theta \vec{x}_{\text{loc}} + (1 - \theta) \vec{x}_{\text{glob}}$ satisfies

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then

$$\begin{aligned} f(\vec{x}_{\text{loc}}) &\leq f(\vec{x}_\theta) \\ &= f(\theta \vec{x}_{\text{loc}} + (1 - \theta) \vec{x}_{\text{glob}}) \end{aligned}$$

Proof

Choose θ so that $\vec{x}_\theta := \theta \vec{x}_{\text{loc}} + (1 - \theta) \vec{x}_{\text{glob}}$ satisfies

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then

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Proof

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then

$$\begin{aligned} f(\vec{x}_{\text{loc}}) &\leq f(\vec{x}_\theta) \\ &= f(\theta \vec{x}_{\text{loc}} + (1 - \theta) \vec{x}_{\text{glob}}) \\ &\leq \theta f(\vec{x}_{\text{loc}}) + (1 - \theta) f(\vec{x}_{\text{glob}}) \quad \text{by convexity of } f \\ &< f(\vec{x}_{\text{loc}}) \quad \text{because } f(\vec{x}_{\text{glob}}) < f(\vec{x}_{\text{loc}}) \end{aligned}$$

Strictly convex functions

Strictly convex functions have at most **one** global minimum

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$$f(0.5\vec{x} + 0.5\vec{y}) < 0.5f(\vec{x}) + 0.5f(\vec{y})$$

Strictly convex functions

Strictly convex functions have at most **one** global minimum

Proof: Assume two minima exist at $\vec{x} \neq \vec{y}$ with value $v_{\min}$

$$\begin{aligned} f(0.5\vec{x} + 0.5\vec{y}) &< 0.5f(\vec{x}) + 0.5f(\vec{y}) \\ &= v_{\min} \end{aligned}$$

Norm

Let $\mathcal{V}$ be a vector space, a norm is a function $||\cdot||$ from $\mathcal{V}$ to $\mathbb{R}$ with the following properties

- ▶ It is **homogeneous**. For any scalar α and any $\vec{x} \in \mathcal{V}$

$$||\alpha \vec{x}|| = |\alpha| ||\vec{x}||.$$

- ▶ It satisfies the **triangle inequality**

$$||\vec{x} + \vec{y}|| \leq ||\vec{x}|| + ||\vec{y}||.$$

In particular, $||\vec{x}|| \geq 0$

- ▶ $||\vec{x}|| = 0$ implies $\vec{x} = \vec{0}$

Norms are convex

For any $\vec{x}, \vec{y} \in \mathbb{R}^n$ and any $\theta \in (0, 1)$

$$\|\theta \vec{x} + (1 - \theta) \vec{y}\|$$

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For any $\vec{x}, \vec{y} \in \mathbb{R}^n$ and any $\theta \in (0, 1)$

$$\begin{aligned} \|\theta \vec{x} + (1 - \theta) \vec{y}\| &\leq \|\theta \vec{x}\| + \|(1 - \theta) \vec{y}\| \\ &= \theta \|\vec{x}\| + (1 - \theta) \|\vec{y}\| \end{aligned}$$

Composition of convex and affine function

If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex, then for any $A \in \mathbb{R}^{n \times m}$ and $\vec{b} \in \mathbb{R}^n$

$$h(\vec{x}) := f(A\vec{x} + \vec{b})$$

is convex

Consequence:

$$f(\vec{x}) := \left\| A\vec{x} + \vec{b} \right\|$$

is convex for any A and $\vec{b}$

Least-squares cost function is convex

Composition of convex and affine function

$$h(\theta \vec{x} + (1 - \theta) \vec{y})$$

Composition of convex and affine function

$$h(\theta \vec{x} + (1 - \theta) \vec{y}) = f\left(\theta \left(A\vec{x} + \vec{b}\right) + (1 - \theta) \left(A\vec{y} + \vec{b}\right)\right)$$

Composition of convex and affine function

$$\begin{aligned}h(\theta \vec{x} + (1 - \theta) \vec{y}) &= f\left(\theta \left(A\vec{x} + \vec{b}\right) + (1 - \theta) \left(A\vec{y} + \vec{b}\right)\right) \\&\leq \theta f\left(A\vec{x} + \vec{b}\right) + (1 - \theta) f\left(A\vec{y} + \vec{b}\right)\end{aligned}$$

Composition of convex and affine function

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ℓ_0 "norm"

Number of **nonzero** entries in a vector

Not a norm!

$$\|2\vec{x}\|_0$$

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$$\|2\vec{x}\|_0 = \|\vec{x}\|_0$$

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$$\begin{aligned} \|2\vec{x}\|_0 &= \|\vec{x}\|_0 \\ &\neq 2 \|\vec{x}\|_0 \end{aligned}$$

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Not convex

Let $\vec{x} := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\vec{y} := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, for any $\theta \in (0, 1)$

$$\|\theta\vec{x} + (1 - \theta)\vec{y}\|_0$$

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$$\|\theta\vec{x} + (1 - \theta)\vec{y}\|_0 = 2$$

$$\theta\|\vec{x}\|_0 + (1 - \theta)\|\vec{y}\|_0$$

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Promoting sparsity

Toy problem: Find t such that

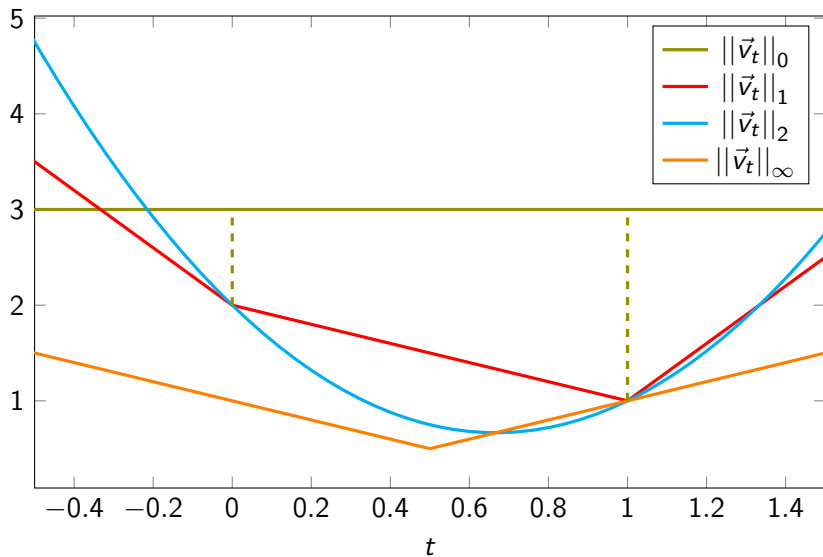
$$\vec{v}_t := \begin{bmatrix} t \\ t - 1 \\ t - 1 \end{bmatrix}$$

is sparse

Strategy: Minimize

$$f(t) := \|\vec{v}_t\|$$

Promoting sparsity



The rank is not convex

The rank of matrices in $\mathbb{R}^{n \times n}$ interpreted as a function from $\mathbb{R}^{n \times n}$ to $\mathbb{R}$ is **not** convex

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$$X := \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad Y := \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

For any $\theta \in (0, 1)$

$$\text{rank}(\theta X + (1 - \theta) Y)$$

$$\theta \text{rank}(X) + (1 - \theta) \text{rank}(Y)$$

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$$\text{rank}(\theta X + (1 - \theta) Y) = 2$$

$$\theta \text{rank}(X) + (1 - \theta) \text{rank}(Y) = 1$$

Matrix norms

Frobenius norm

$$\|A\|_F := \sqrt{\sum_{i=1}^m \sum_{j=1}^n A_{ij}^2} = \sqrt{\sum_{i=1}^{\min\{m,n\}} \sigma_i^2}$$

Operator norm

$$\|A\| := \max_{\{\|\vec{x}\|_2=1 \mid \vec{x} \in \mathbb{R}^n\}} \|A\vec{x}\|_2 = \sigma_1$$

Nuclear norm

$$\|A\|_* := \sum_{i=1}^{\min\{m,n\}} \sigma_i$$

Hölder's inequality for matrices

For any matrix $A \in \mathbb{R}^{m \times n}$,

$$\|A\|_* = \sup_{\{\|B\| \leq 1 \mid B \in \mathbb{R}^{m \times n}\}} \langle A, B \rangle .$$

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Consequence: nuclear norm satisfies **triangle inequality**

$$\|A + B\|_* = \sup_{\{\|C\| \leq 1 \mid C \in \mathbb{R}^{m \times n}\}} \langle A + B, C \rangle$$

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Promoting low-rank structure

Finding low-rank matrices consistent with data is often very useful

Toy problem: Find t such that

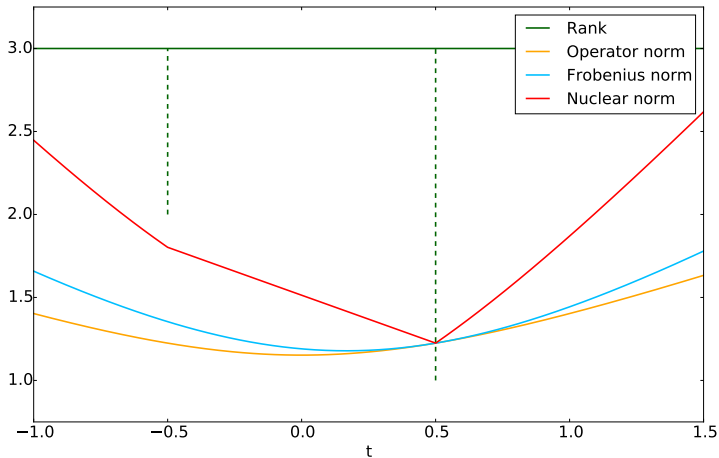
$$M(t) := \begin{bmatrix} 0.5 + t & 1 & 1 \\ 0.5 & 0.5 & t \\ 0.5 & 1 - t & 0.5 \end{bmatrix},$$

is low rank

Strategy: Minimize

$$f(t) := ||M(t)||$$

Promoting low-rank structure



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Gradient

$$\nabla f(\vec{x}) = \begin{bmatrix} \frac{\partial f(\vec{x})}{\partial \vec{x}[1]} \\ \frac{\partial f(\vec{x})}{\partial \vec{x}[2]} \\ \dots \\ \frac{\partial f(\vec{x})}{\partial \vec{x}[n]} \end{bmatrix}$$

If the gradient exists at every point, the function is said to be **differentiable**

Directional derivative

Encodes first-order rate of change in a particular direction

$$\begin{aligned} f'_{\vec{u}}(\vec{x}) &:= \lim_{h \rightarrow 0} \frac{f(\vec{x} + h\vec{u}) - f(\vec{x})}{h} \\ &= \langle \nabla f(\vec{x}), \vec{u} \rangle \end{aligned}$$

where $\|\vec{u}\|_2 = 1$

Direction of maximum variation

∇f is direction of maximum increase

$-\nabla f$ is direction of maximum decrease

$$|f'_{\vec{u}}(\vec{x})| = \left| \nabla f(\vec{x})^T \vec{u} \right|$$

Direction of maximum variation

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$$\begin{aligned} |f'_{\vec{u}}(\vec{x})| &= \left| \nabla f(\vec{x})^T \vec{u} \right| \\ &\leq \|\nabla f(\vec{x})\|_2 \|\vec{u}\|_2 \end{aligned} \quad \text{Cauchy-Schwarz inequality}$$

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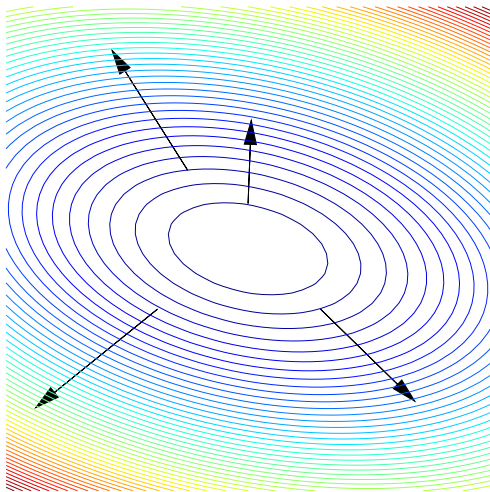
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equality holds if and only if $\vec{u} = \pm \frac{\nabla f(\vec{x})}{\|\nabla f(\vec{x})\|_2}$

Gradient



Gradients of simple functions

Let $A \in \mathbb{R}^{a \times b}$, $M \in \mathbb{R}^{b \times b}$ and symmetric, $\vec{x} \in \mathbb{R}^b, \vec{c} \in \mathbb{R}^b$, $d \in \mathbb{R}$

$$f_1(\vec{x}) := d,$$

$$f_2(\vec{x}) := \vec{c}^T \vec{x},$$

$$f_3(\vec{x}) := \vec{x}^T M \vec{x},$$

$$\nabla f_1(\vec{x}) =$$

$$\nabla f_2(\vec{x}) =$$

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Gradients of simple functions

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$$f_3(\vec{x}) := \vec{x}^T M \vec{x},$$

$$\nabla f_1(\vec{x}) = 0$$

$$\nabla f_2(\vec{x}) = \vec{c}$$

$$\nabla f_3(\vec{x}) = 2M\vec{x}$$

Least squares

Let $\vec{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\vec{\beta} \in \mathbb{R}^p$

The gradient of the least-squares cost function

$$f(\vec{\beta}) := \frac{1}{2} \left\| \vec{y} - X\vec{\beta} \right\|_2^2 = \frac{1}{2} \vec{y}^T \vec{y} + \frac{1}{2} \vec{\beta}^T X^T X \vec{\beta} - \vec{y}^T X \vec{\beta}$$

equals

$$\nabla f(\vec{\beta}) =$$

Least squares

Let $\vec{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\vec{\beta} \in \mathbb{R}^p$

The gradient of the least-squares cost function

$$f(\vec{\beta}) := \frac{1}{2} \left\| \vec{y} - X\vec{\beta} \right\|_2^2 = \frac{1}{2} \vec{y}^T \vec{y} + \frac{1}{2} \vec{\beta}^T X^T X \vec{\beta} - \vec{y}^T X \vec{\beta}$$

equals

$$\nabla f(\vec{\beta}) = X^T (X\vec{\beta} - \vec{y})$$

First-order approximation

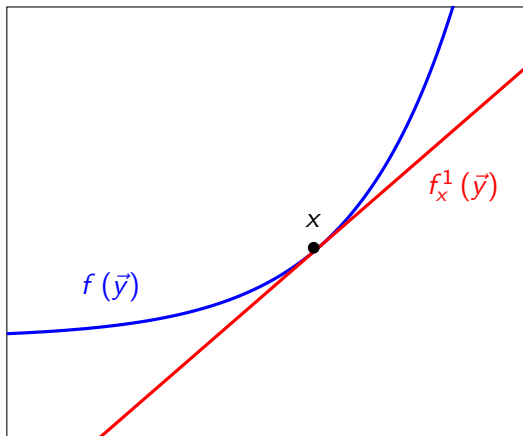
The first-order or linear approximation of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ at $\vec{x}$ is

$$f_{\vec{x}}^1(\vec{y}) := f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x})$$

If f is differentiable at $\vec{x}$

$$\lim_{\vec{y} \rightarrow \vec{x}} \frac{f(\vec{y}) - f_{\vec{x}}^1(\vec{y})}{\|\vec{y} - \vec{x}\|_2} = 0$$

First-order approximation



Convexity

A differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if and only if for every $\vec{x}, \vec{y} \in \mathbb{R}^n$

$$f(\vec{y}) \geq f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x})$$

It is strictly convex if and only if

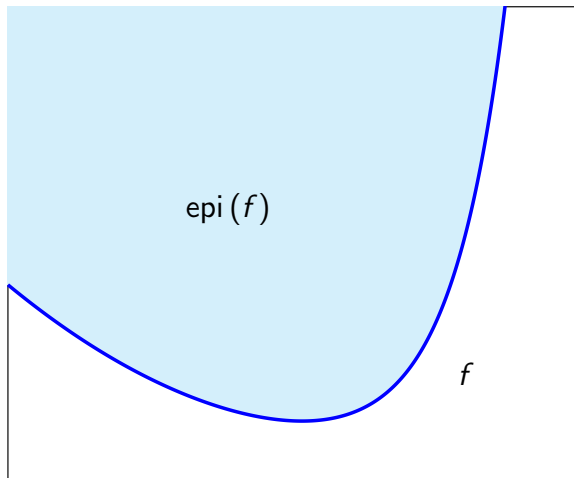
$$f(\vec{y}) > f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x})$$

Epigraph

The epigraph of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is

$$\text{epi}(f) := \left\{ \vec{x} \mid f \left(\begin{bmatrix} \vec{x}[1] \\ \vdots \\ \vec{x}[n] \end{bmatrix} \right) \leq \vec{x}[n+1] \right\}$$

Epigraph



Supporting hyperplane

A hyperplane $\mathcal{H}$ is a supporting hyperplane of a set $\mathcal{S}$ at $\vec{x}$ if

- ▶ $\mathcal{H}$ and $\mathcal{S}$ **intersect** at $\vec{x}$
- ▶ $\mathcal{S}$ is contained in one of the half-spaces bounded by $\mathcal{H}$

Geometric intuition

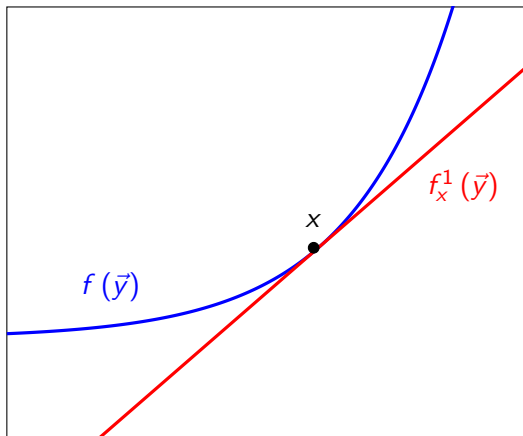
Geometrically, f is convex if and only if for every $\vec{x}$ the plane

$$\mathcal{H}_{f,\vec{x}} := \left\{ \vec{y} \mid \vec{y}[n+1] = f_{\vec{x}}^1 \left(\begin{bmatrix} \vec{y}[1] \\ \vdots \\ \vec{y}[n] \end{bmatrix} \right) \right\}$$

is a supporting hyperplane of the epigraph at $\vec{x}$

If $\nabla f(\vec{x}) = 0$ the hyperplane is **horizontal**

Convexity



Optimality condition

If f is convex, $\nabla f(\vec{x}) = 0$ if and only if $\vec{x}$ is a minimum

For any $\vec{y}$

$$\begin{aligned} f(\vec{y}) &\geq f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x}) \\ &\geq f(\vec{x}) \end{aligned}$$

Least squares

Let $\vec{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\vec{\beta} \in \mathbb{R}^p$

$$f(\vec{\beta}) := \frac{1}{2} \left\| \vec{y} - X\vec{\beta} \right\|_2^2$$
$$\nabla f(\vec{\beta}) = X^T (X\vec{\beta} - \vec{y})$$

Setting gradient to zero yields normal equations

$$X^T X \vec{\beta} = X^T \vec{y}$$

Least squares

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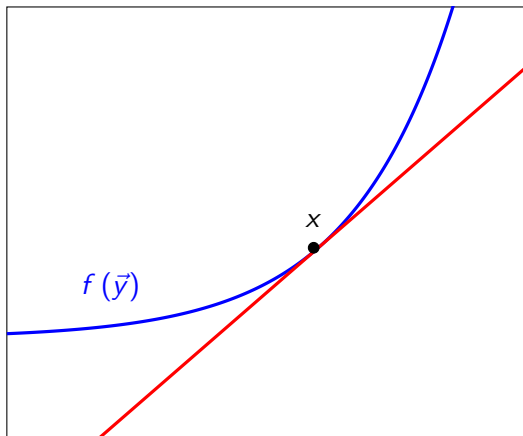
If $X^T X$ is invertible $\vec{\beta}_{\text{LS}} := (X^T X)^{-1} X^T \vec{y}$

Gradient

A differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if and only if for every $\vec{x}, \vec{y} \in \mathbb{R}^n$

$$f(\vec{y}) \geq f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x})$$

Gradient



Subgradient

The **subgradient** of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ at $\vec{x} \in \mathbb{R}^n$ is a vector $\vec{g} \in \mathbb{R}^n$ such that

$$f(\vec{y}) \geq f(\vec{x}) + \vec{g}^T (\vec{y} - \vec{x}), \quad \text{for all } \vec{y} \in \mathbb{R}^n$$

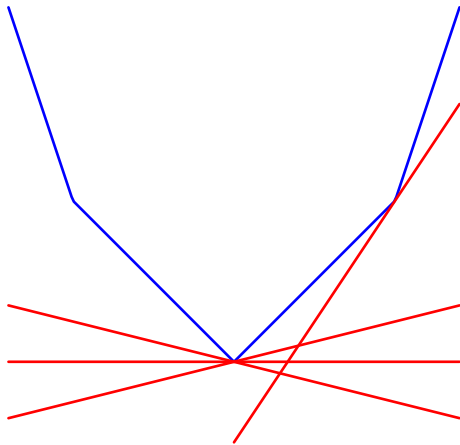
Geometrically, the hyperplane

$$\mathcal{H}_{\vec{g}} := \left\{ \vec{y} \mid \vec{y}[n+1] = \vec{g}^T \begin{pmatrix} \vec{y}[1] \\ \vdots \\ \vec{y}[n] \end{pmatrix} \right\}$$

is a supporting hyperplane of the epigraph at $\vec{x}$

The set of all subgradients at $\vec{x}$ is called the **subdifferential**

Subgradients



Subgradient of differentiable function

If a function is differentiable, the **only** subgradient at each point is the **gradient**

Proof

Assume $\vec{g}$ is a subgradient at $\vec{x}$, for any $\alpha \geq 0$

$$f(\vec{x} + \alpha \vec{e}_i) \geq f(\vec{x}) + \vec{g}^T \alpha \vec{e}_i$$

$$= f(\vec{x}) + \vec{g}[i] \alpha$$

$$f(\vec{x}) \leq f(\vec{x} - \alpha \vec{e}_i) + \vec{g}^T \alpha \vec{e}_i$$

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Combining both inequalities

$$\frac{f(\vec{x}) - f(\vec{x} - \alpha \vec{e}_i)}{\alpha} \leq \vec{g}[i] \leq \frac{f(\vec{x} + \alpha \vec{e}_i) - f(\vec{x})}{\alpha}$$

Proof

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Combining both inequalities

$$\frac{f(\vec{x}) - f(\vec{x} - \alpha \vec{e}_i)}{\alpha} \leq \vec{g}[i] \leq \frac{f(\vec{x} + \alpha \vec{e}_i) - f(\vec{x})}{\alpha}$$

Letting $\alpha \rightarrow 0$, implies $\vec{g}[i] = \frac{\partial f(\vec{x})}{\partial \vec{x}[i]}$

Subgradient

A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if and only if it has a subgradient at every point

It is strictly convex if and only for all $\vec{x} \in \mathbb{R}^n$ there exists $\vec{g} \in \mathbb{R}^n$ such that

$$f(\vec{y}) > f(\vec{x}) + \vec{g}^T (\vec{y} - \vec{x}), \quad \text{for all } \vec{y} \neq \vec{x}.$$

Optimality condition for nondifferentiable functions

$\vec{x}$ is a minimum of f if and only if the zero vector is a subgradient of f at $\vec{x}$

$$f(\vec{y}) \geq f(\vec{x}) + \vec{0}^T (\vec{y} - \vec{x})$$

Optimality condition for nondifferentiable functions

$\vec{x}$ is a minimum of f if and only if the zero vector is a subgradient of f at $\vec{x}$

$$\begin{aligned} f(\vec{y}) &\geq f(\vec{x}) + \vec{0}^T (\vec{y} - \vec{x}) \\ &= f(\vec{x}) \end{aligned}$$

for all $\vec{y} \in \mathbb{R}^n$

Sum of subgradients

Let $\vec{g}_1$ and $\vec{g}_2$ be subgradients at $\vec{x} \in \mathbb{R}^n$ of $f_1 : \mathbb{R}^n \rightarrow \mathbb{R}$ and $f_2 : \mathbb{R}^n \rightarrow \mathbb{R}$

$\vec{g} := \vec{g}_1 + \vec{g}_2$ is a subgradient of $f := f_1 + f_2$ at $\vec{x}$

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Proof: For any $\vec{y} \in \mathbb{R}^n$

$$f(\vec{y}) = f_1(\vec{y}) + f_2(\vec{y})$$

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Subgradient of scaled function

Let $\vec{g}_1$ be a subgradient at $\vec{x} \in \mathbb{R}^n$ of $f_1 : \mathbb{R}^n \rightarrow \mathbb{R}$

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Proof: For any $\vec{y} \in \mathbb{R}^n$

$$\begin{aligned} f_2(\vec{y}) &= \alpha f_1(\vec{y}) \\ &\geq \alpha \left(f_1(\vec{x}) + \vec{g}_1^T (\vec{y} - \vec{x}) \right) \end{aligned}$$

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Subdifferential of absolute value

At $x \neq 0$, $f(x) = |x|$ is differentiable, so $g = \text{sign}(x)$

At $x = 0$, we need

$$f(0 + y) \geq f(0) + g(y - 0)$$

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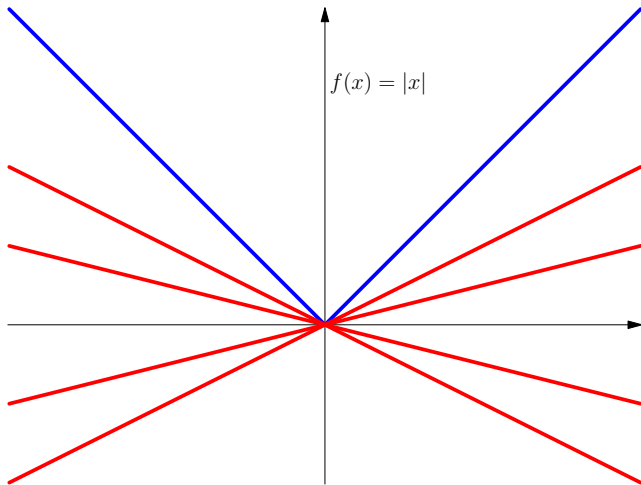
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$$|y| \geq gy$$

Holds if and only if $|g| \leq 1$

Subdifferential of absolute value



Subdifferential of ℓ_1 norm

$\vec{g}$ is a subgradient of the ℓ_1 norm at $\vec{x} \in \mathbb{R}^n$ if and only if

$$\vec{g}[i] = \text{sign}(x[i]) \quad \text{if } x[i] \neq 0$$

$$|\vec{g}[i]| \leq 1 \quad \text{if } \vec{x}[i] = 0$$

Proof (one direction)

$$\|\vec{y}\|_1 \geq \langle g, \vec{y} \rangle \quad \text{by Hölder's inequality because } \|g\|_\infty \leq 1$$

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$$\begin{aligned} \|\vec{y}\|_1 &\geq \langle g, \vec{y} \rangle \quad \text{by Hölder's inequality because } \|g\|_\infty \leq 1 \\ &= \langle g, \vec{x} \rangle + \langle g, \vec{y} - \vec{x} \rangle \end{aligned}$$

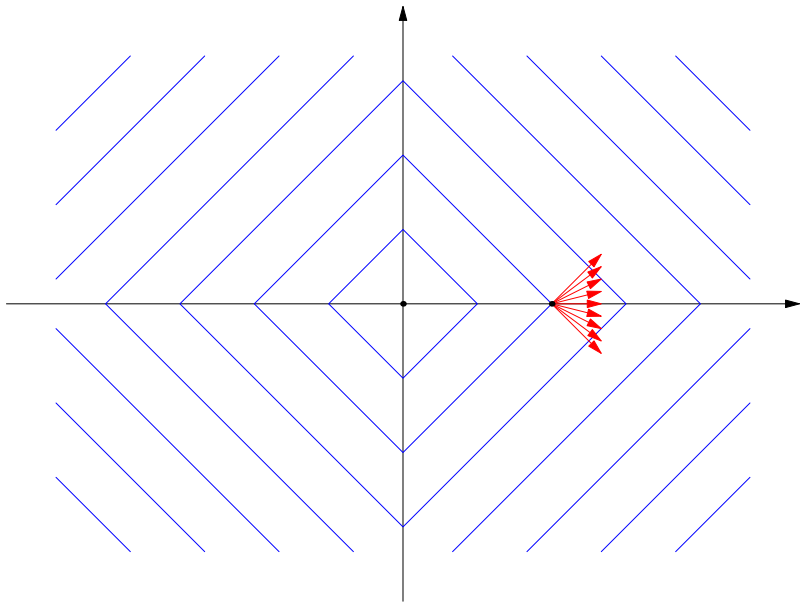
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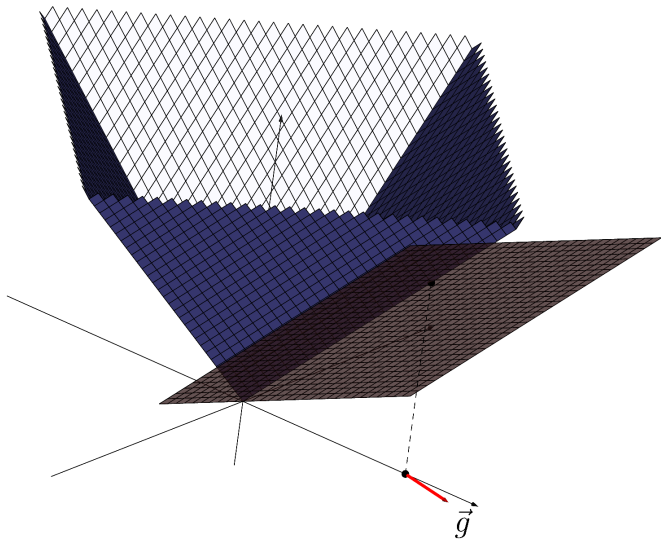
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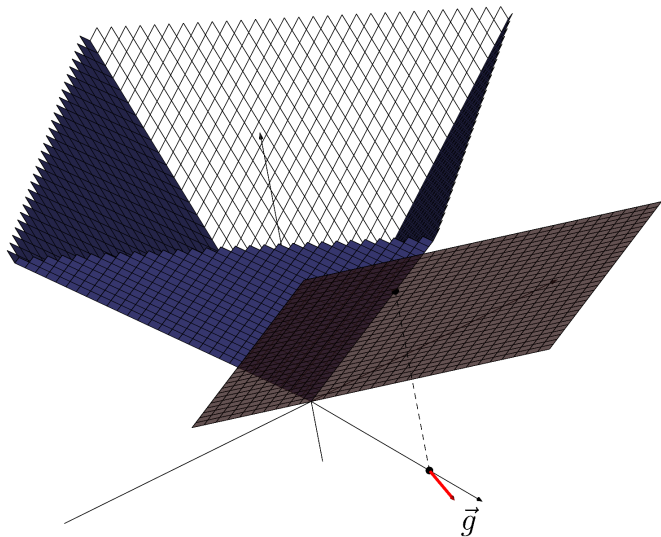
Subdifferential of ℓ_1 norm



Subdifferential of ℓ_1 norm



Subdifferential of ℓ_1 norm



Subdifferential of the nuclear norm

Let $X \in \mathbb{R}^{m \times n}$ be a rank- r matrix with SVD USV^T , where $U \in \mathbb{R}^{m \times r}$, $V \in \mathbb{R}^{n \times r}$ and $S \in \mathbb{R}^{r \times r}$

A matrix G is a subgradient of the nuclear norm at X if and only if

$$G := UV^T + W$$

where W satisfies

$$\|W\| \leq 1$$

$$U^T W = 0$$

$$W V = 0$$

Proof

Analogy with ℓ_1 norm

- ▶ ℓ_1 norm $\rightarrow$ nuclear norm
- ▶ ℓ_∞ norm $\rightarrow$ operator norm
- ▶ $UV^T \rightarrow$ sign vector

Proof

First step: prove that $\|G\| \leq 1$

By Pythagoras' Theorem, for any $\vec{x} \in \mathbb{R}^m$ with unit ℓ_2 norm we have

$$\left\| \mathcal{P}_{\text{row}(X)} \vec{x} \right\|_2^2 + \left\| \mathcal{P}_{\text{row}(X)^\perp} \vec{x} \right\|_2^2 = \|\vec{x}\|_2^2 = 1$$

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The rows of UV^T are in $\text{row}(X)$ and the rows of W in $\text{row}(X)^\perp$, so

$$\|G\|^2 := \max_{\{\|\vec{x}\|_2=1 \mid \vec{x} \in \mathbb{R}^n\}} \|G \vec{x}\|_2^2$$

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Hölder's inequality for matrices

Hölder's inequality:

$$\|\vec{x}\|_1 = \sup_{\{\|\vec{y}\|_\infty \leq 1 \mid \vec{y} \in \mathbb{R}^n\}} \langle \vec{x}, \vec{y} \rangle$$

For any matrix $A \in \mathbb{R}^{m \times n}$,

$$\|A\|_* = \sup_{\{\|B\| \leq 1 \mid B \in \mathbb{R}^{m \times n}\}} \langle A, B \rangle$$

Proof

For any matrix $Y \in \mathbb{R}^{m \times n}$

$$\begin{aligned}\|Y\|_* &\geq \langle G, Y \rangle \\ &= \langle G, X \rangle + \langle G, Y - X \rangle \\ &= \langle UV^T, X \rangle + \langle W, X \rangle + \langle G, Y - X \rangle\end{aligned}$$

Proof

$$U^T W = 0 \text{ implies } \langle W, X \rangle = \langle W, USV^T \rangle = \langle U^T W, SV^T \rangle = 0$$

Proof

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Proof

$$\langle UV^T, X \rangle$$

Proof

$$\langle UV^T, X \rangle = \text{tr}(VU^T X)$$

Proof

$$\begin{aligned}\langle UV^T, X \rangle &= \text{tr}(VU^T X) \\ &= \text{tr}(VU^T USV^T)\end{aligned}$$

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Proof

$$\begin{aligned}\langle UV^T, X \rangle &= \text{tr}(VU^T X) \\ &= \text{tr}(VU^T USV^T) \\ &= \text{tr}(V^T V S) \\ &= \text{tr}(S) \\ &= \|X\|_*\end{aligned}$$

Proof

For any matrix $Y \in \mathbb{R}^{m \times n}$

$$\begin{aligned}\|Y\|_* &\geq \langle G, Y \rangle \\ &= \langle G, X \rangle + \langle G, Y - X \rangle \\ &= \langle UV^T, X \rangle + \langle G, Y - X \rangle \\ &= \langle UV^T, X \rangle + \langle W, X \rangle + \langle G, Y - X \rangle \\ &= \|X\|_* + \langle G, Y - X \rangle\end{aligned}$$

Motivating applications

Convex functions

Optimality conditions

Convex Regularization

Optimization algorithms

Sparse regression

Linear regression is challenging when the number of features p is large

Problem: How to choose subset of features $\mathcal{I} \subset \{1, \dots, p\}$, such that

$$y \approx \sum_{i \in \mathcal{I}} \vec{\beta}[i] \vec{x}[i] + \beta_0$$

Equivalently, find sparse coefficient vector $\vec{\beta} \in \mathbb{R}^p$ such that

$$y \approx \langle \vec{x}, \vec{\beta} \rangle + \beta_0$$

Sparse linear regression

Find a small subset of useful features

Model selection problem

Two objectives:

- ▶ Good fit to the data; $\left\|X\vec{\beta} - \vec{y}\right\|_2^2$ should be as small as possible
- ▶ Using a small number of features; $\vec{\beta}$ should be as sparse as possible

The lasso

Uses ℓ_1 -norm regularization to promote sparse coefficients

$$\vec{\beta}_{\text{lasso}} := \arg \min_{\vec{\beta}} \frac{1}{2} \left\| \vec{y} - X\vec{\beta} \right\|_2^2 + \lambda \left\| \vec{\beta} \right\|_1$$

Nonnegative weighted sums

The weighted sum of m convex functions $f_1, \dots, f_m$

$$f := \sum_{i=1}^m \alpha_i f_i$$

is convex if $\alpha_1, \dots, \alpha_m \in \mathbb{R}$ are nonnegative

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The weighted sum of m convex functions $f_1, \dots, f_m$

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is convex if $\alpha_1, \dots, \alpha_m \in \mathbb{R}$ are nonnegative

Proof:

$$f(\theta \vec{x} + (1 - \theta) \vec{y})$$

Nonnegative weighted sums

The weighted sum of m convex functions $f_1, \dots, f_m$

$$f := \sum_{i=1}^m \alpha_i f_i$$

is convex if $\alpha_1, \dots, \alpha \in \mathbb{R}$ are nonnegative

Proof:

$$f(\theta \vec{x} + (1 - \theta) \vec{y}) = \sum_{i=1}^m \alpha_i f_i(\theta \vec{x} + (1 - \theta) \vec{y})$$

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$$\begin{aligned} f(\theta \vec{x} + (1 - \theta) \vec{y}) &= \sum_{i=1}^m \alpha_i f_i(\theta \vec{x} + (1 - \theta) \vec{y}) \\ &\leq \sum_{i=1}^m \alpha_i (\theta f_i(\vec{x}) + (1 - \theta) f_i(\vec{y})) \end{aligned}$$

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Regularized least-squares

Regularized least-squares cost functions

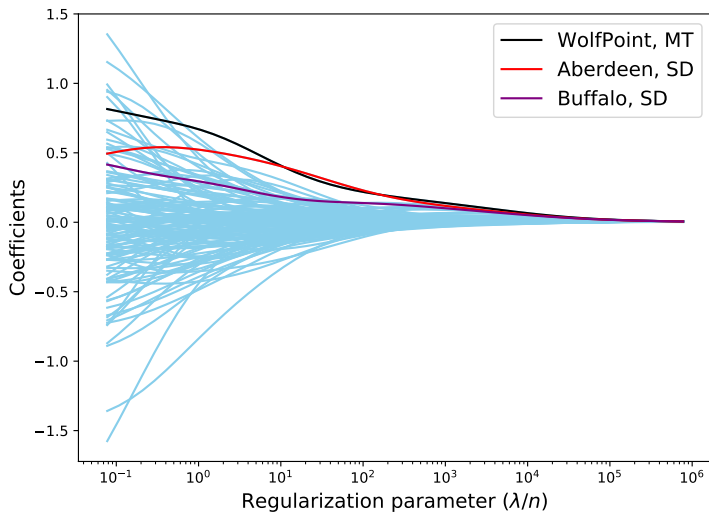
$$||A\vec{x} - \vec{y}||_2^2 + ||\vec{x}'||$$

are convex

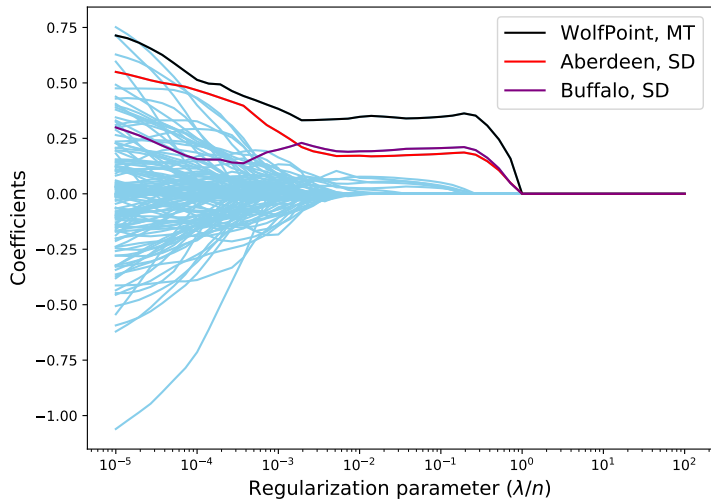
Temperature prediction via linear regression

- ▶ Dataset of hourly temperatures measured at weather stations all over the US
- ▶ Goal: Predict temperature in Jamestown (North Dakota) from other temperatures
- ▶ Response: Temperature in Jamestown
- ▶ Features: Temperatures in 133 other stations ($p = 133$) in 2015
- ▶ Test set: 10^3 measurements
- ▶ Additional test set: All measurements from 2016

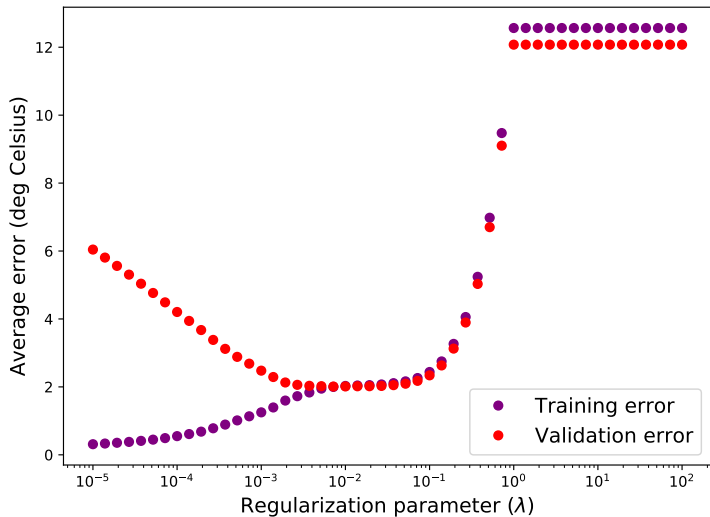
Ridge regression $n := 135$



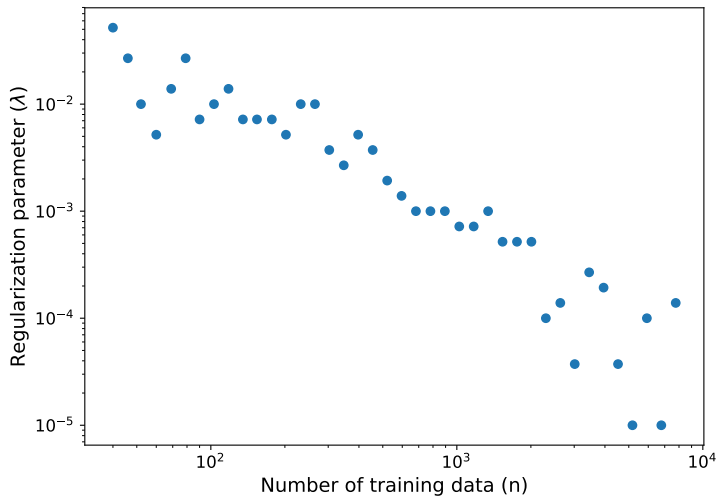
Lasso $n := 135$



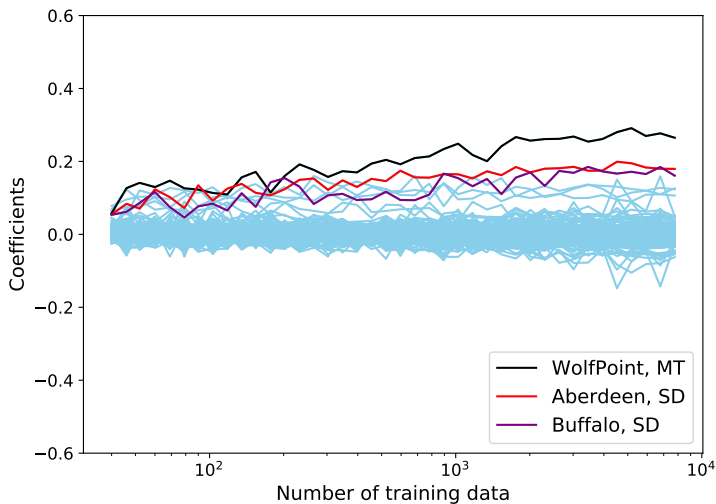
Lasso $n := 135$



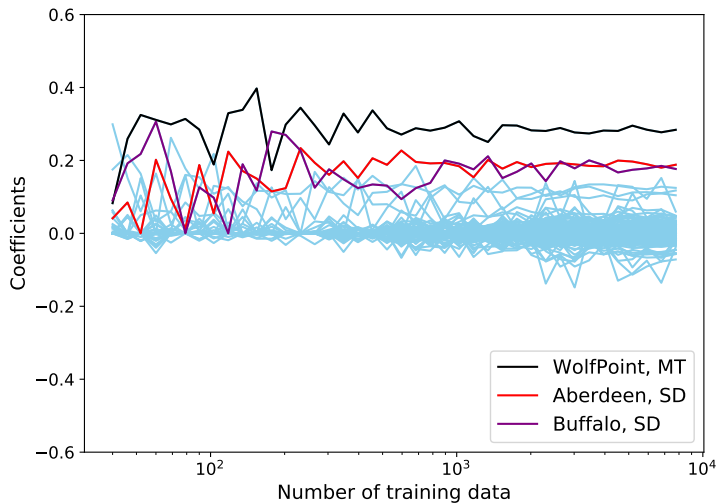
Lasso $n := 135$



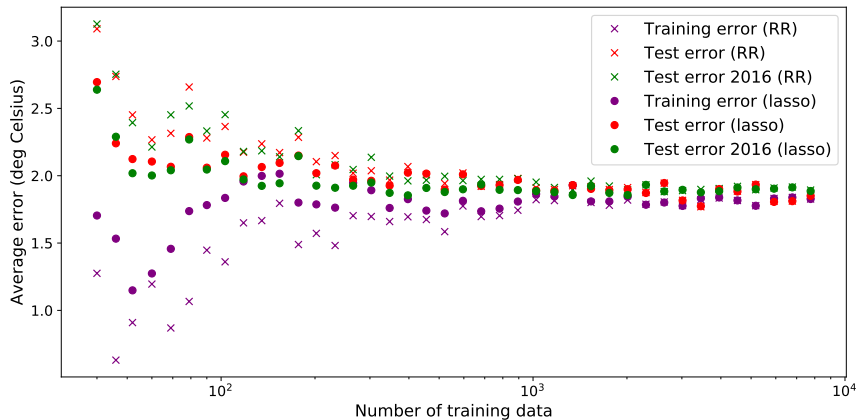
Ridge-regression coefficients



Lasso coefficients



Results



Proximal operator

Linear combination of function and least-squares term

$$\text{prox}_f(\vec{y}) := \arg \min_{\vec{x}} f(\vec{x}) + \frac{1}{2} \|\vec{x} - \vec{y}\|_2^2$$

Proximal operator of ℓ_2 norm

The proximal operator of the squared ℓ_2 norm is

$$\text{prox}_{\alpha \|\cdot\|_2^2}(\vec{y}) = \frac{\vec{y}}{1 + 2\alpha}$$

for all $\alpha > 0$

Proof

The gradient of the function

$$\begin{aligned} f(\vec{x}) &:= \alpha \|\vec{x}\|_2^2 + \frac{1}{2} \|\vec{x} - \vec{y}\|_2^2 \\ &= \left(\frac{1}{2} + \alpha\right) \vec{x}^T \vec{x} + \frac{1}{2} \vec{y}^T \vec{y} - \vec{y}^T \vec{x} \end{aligned}$$

equals

$$\nabla f(\vec{x}) =$$

Proof

The gradient of the function

$$\begin{aligned} f(\vec{x}) &:= \alpha \|\vec{x}\|_2^2 + \frac{1}{2} \|\vec{x} - \vec{y}\|_2^2 \\ &= \left(\frac{1}{2} + \alpha\right) \vec{x}^T \vec{x} + \frac{1}{2} \vec{y}^T \vec{y} - \vec{y}^T \vec{x} \end{aligned}$$

equals

$$\nabla f(\vec{x}) = (1 + 2\alpha) \vec{x} - \vec{y}$$

Proximal operator of ℓ_1 norm

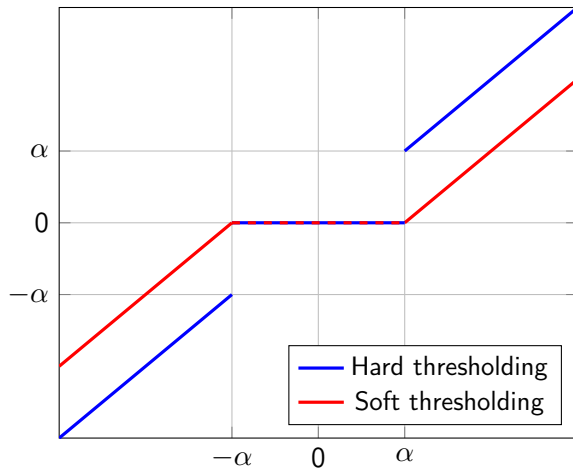
The proximal operator of the ℓ_1 norm is the **soft-thresholding operator**

$$\text{prox}_{\alpha \|\cdot\|_1}(y) = \mathcal{S}_\alpha(y)$$

where $\alpha > 0$ and

$$\mathcal{S}_\alpha(y)_i := \begin{cases} y_i - \text{sign}(y_i) \alpha & \text{if } |y_i| \geq \alpha \\ 0 & \text{otherwise} \end{cases}$$

Thresholding



Proof

The subgradients of the function

$$f(\vec{x}) := \alpha \|\vec{x}\|_1 + \frac{1}{2} \|\vec{x} - \vec{y}\|_2^2$$

at $\vec{x}$ equal

$$\vec{g}_{\text{prox}} = \alpha \vec{g}_{\ell_1}(\vec{x}) + \vec{x} - \vec{y}$$

where $\vec{g}_{\ell_1}(\vec{x})$ is any subgradient of the ℓ_1 norm at $\vec{x}$

Setting it to zero

$$\vec{x}_{\min} + \alpha \vec{g}_{\ell_1}(\vec{x}_{\min}) = \vec{y}$$

Proof

If $|\vec{y}[j]| \geq \alpha$

$$\vec{x}_{\min}[j] = \vec{y}[j] - \alpha \vec{g}_{\ell_1}(\vec{x}_{\min})[j]$$

Proof

If $|\vec{y}[j]| \geq \alpha$

$$\begin{aligned}\vec{x}_{\min}[j] &= \vec{y}[j] - \alpha \vec{g}_{\ell_1}(\vec{x}_{\min})[j] \\ &= \vec{y}[j] - \alpha \operatorname{sign}(\vec{x}[j])\end{aligned}$$

Proof

If $|\vec{y}[j]| \geq \alpha$

$$\begin{aligned}\vec{x}_{\min}[j] &= \vec{y}[j] - \alpha \vec{g}_{\ell_1}(\vec{x}_{\min})[j] \\ &= \vec{y}[j] - \alpha \operatorname{sign}(\vec{x}[j])\end{aligned}$$

If $|\vec{y}[j]| < \alpha$ the only possible solution is zero

Linear regression with orthonormal features

Let $U \in \mathbb{R}^{n \times p}$ be a matrix with orthonormal columns and $\vec{y} \in \mathbb{R}^n$

For any f

$$\arg \min_{\vec{\beta}} \frac{1}{2} \left\| \vec{y} - U\vec{\beta} \right\|_2^2 + f(\vec{\beta}) = \arg \min_{\vec{\beta}} \frac{1}{2} \left\| U^T \vec{y} - \vec{\beta} \right\|_2^2 + f(\vec{\beta}).$$

Proof

$$\frac{1}{2} \left\| \vec{y} - U\vec{\beta} \right\|_2^2 + f(\vec{\beta}) = \frac{1}{2} \vec{\beta}^T U^T U \vec{\beta} + \frac{1}{2} \vec{y}^T \vec{y} - \vec{y}^T U \vec{\beta} + f(\vec{\beta})$$

Proof

$$\begin{aligned}\frac{1}{2} \left\| \vec{y} - U\vec{\beta} \right\|_2^2 + f(\vec{\beta}) &= \frac{1}{2} \vec{\beta}^T U^T U \vec{\beta} + \frac{1}{2} \vec{y}^T \vec{y} - \vec{y}^T U \vec{\beta} + f(\vec{\beta}) \\ &= \frac{1}{2} \vec{\beta}^T \vec{\beta} + \frac{1}{2} \vec{y}^T \vec{y} - (U^T \vec{y})^T \vec{\beta} + f(\vec{\beta})\end{aligned}$$

Proof

$$\begin{aligned}\frac{1}{2} \left\| \vec{y} - U\vec{\beta} \right\|_2^2 + f(\vec{\beta}) &= \frac{1}{2} \vec{\beta}^T U^T U \vec{\beta} + \frac{1}{2} \vec{y}^T \vec{y} - \vec{y}^T U \vec{\beta} + f(\vec{\beta}) \\ &= \frac{1}{2} \vec{\beta}^T \vec{\beta} + \frac{1}{2} \vec{y}^T \vec{y} - (U^T \vec{y})^T \vec{\beta} + f(\vec{\beta}) \\ &= \frac{1}{2} \left\| U^T \vec{y} - \vec{\beta} \right\|_2^2 + f(\vec{\beta}) + \frac{1}{2} \vec{y}^T \vec{y} - \frac{1}{2} \vec{y}^T U U^T \vec{y}\end{aligned}$$

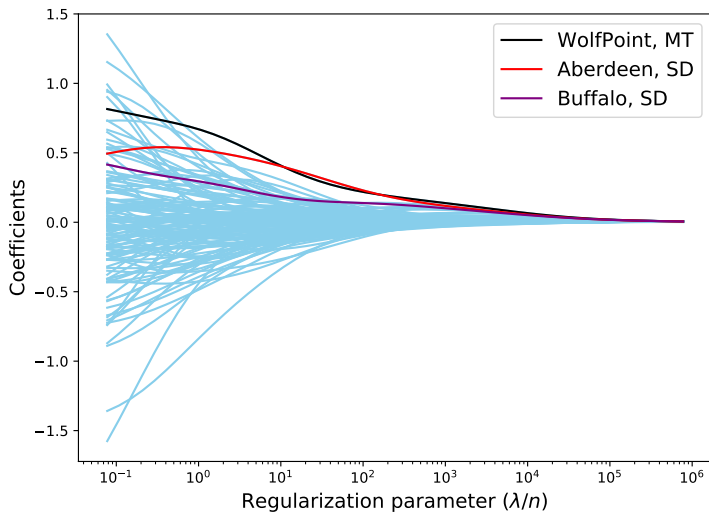
Consequence

$U^T \vec{y}$ is the least-squares solution

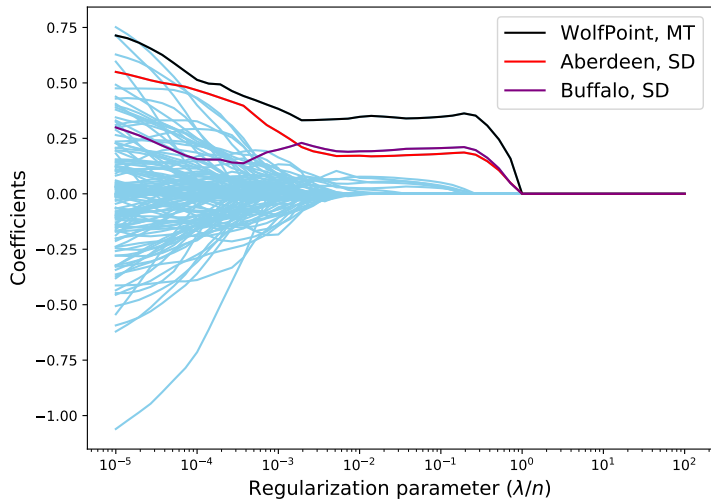
Ridge regression scales all entries equally

The lasso soft-thresholds the entries

Ridge regression $n := 135$



Lasso $n := 135$



Collaborative filtering

							...
	★★★★★	?	★★★★☆	?	?	?	...
	?	★★★★☆	?	?	★★★★☆	?	...
	?	?	?	★★★★☆	★★★★☆	?	...
	?	★★★★☆	★★★★☆	?	?	★★★★★	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Low-rank matrix estimation

If all entries are observed, truncating the SVD is optimal

Let USV^T be the SVD of a matrix $A \in \mathbb{R}^{m \times n}$

The truncated SVD $U_{:,1:r}S_{1:r,1:r}V_{:,1:r}^T$ is the best rank- r approximation

$$U_{:,1:r}S_{1:r,1:r}V_{:,1:r}^T = \arg \min_{\{\tilde{A} \mid \text{rank}(\tilde{A})=r\}} \left\| A - \tilde{A} \right\|_F$$

Low-rank matrix estimation

First idea:

$$\min_{X \in \mathbb{R}^{m \times n}} \text{rank}(X) \quad \text{such that } X_{\Omega} = \vec{y}$$

Ω : indices of revealed entries

$\vec{y}$: revealed entries

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Computationally intractable because of missing entries

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Computationally intractable because of missing entries

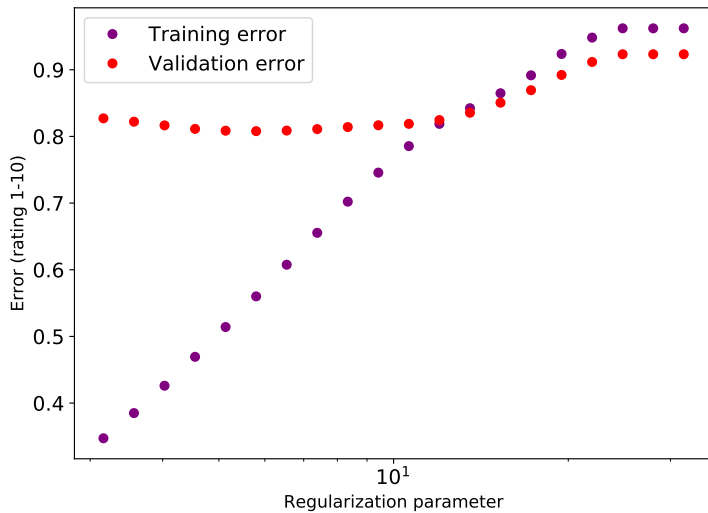
Tractable alternative:

$$\min_{X \in \mathbb{R}^{n_1 \times n_2}} \frac{1}{2} \|X_{\Omega} - \vec{y}\|_2^2 + \lambda \|X\|_*$$

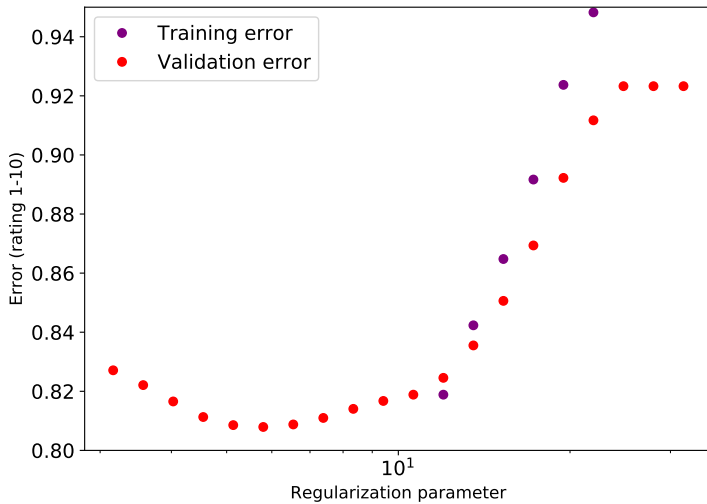
Collaborative filtering

- ▶ Movielens data
- ▶ Ratings between 1 and 10
- ▶ 100 users and movies with more ratings
- ▶ 6,031 out of 10^4 ratings are observed
- ▶ Test set with 10^3
- ▶ Validation set with $\max\{n_{\text{train}}, 400\}$

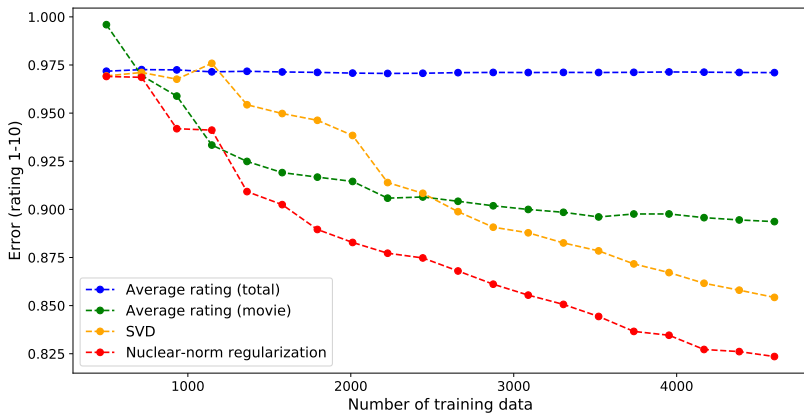
$n_{\text{train}} := 4,600$



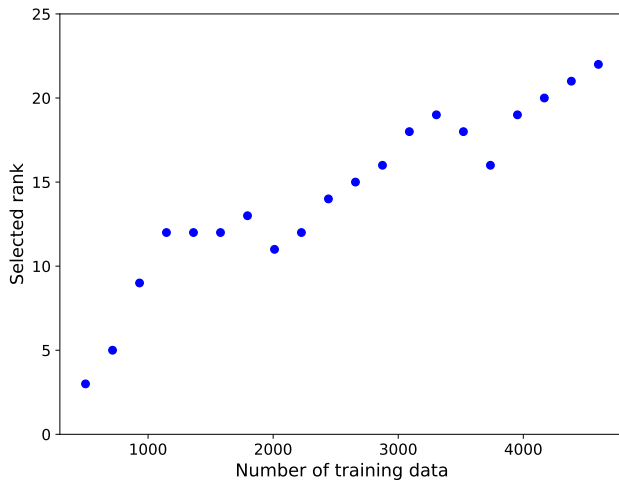
$n_{\text{train}} := 4,600$



Results



Rank



Proximal operator of nuclear norm

The solution X to

$$\min_{X \in \mathbb{R}^{m \times n}} \frac{1}{2} \|Y - X\|_F^2 + \alpha \|X\|_*$$

is obtained by **soft-thresholding** the SVD of Y

$$X_{\text{prox}} = \mathcal{D}_\alpha(Y)$$

$$\mathcal{D}_\alpha(M) := U \mathcal{S}_\alpha(S) V^T \quad \text{where } M = U S V^T$$

$$\mathcal{S}_\alpha(S)_{ii} := \begin{cases} S_{ii} - \alpha & \text{if } S_{ii} > \alpha \\ 0 & \text{otherwise} \end{cases}$$

Proximal operator of nuclear norm

The subgradients of

$$\frac{1}{2} \|X - Y\|_F^2 + \alpha \|X\|_*$$

are of the form

$$X - Y + \alpha G$$

where G is a subgradient of the nuclear norm at X

$\mathcal{D}_\alpha(Y)$ is a minimizer if and only if

$$G = \frac{1}{\alpha} (Y - D_\alpha(Y))$$

is a subgradient of the nuclear norm at $\mathcal{D}_\alpha(Y)$

Subdifferential of the nuclear norm

Let $X \in \mathbb{R}^{m \times n}$ be a rank- r matrix with SVD USV^T , where $U \in \mathbb{R}^{m \times r}$, $V \in \mathbb{R}^{n \times r}$ and $S \in \mathbb{R}^{r \times r}$

A matrix G is a subgradient of the nuclear norm at X if and only if

$$G := UV^T + W$$

where W satisfies

$$\|W\| \leq 1$$

$$U^T W = 0$$

$$W V = 0$$

Proximal operator of nuclear norm

Separate SVD of Y into singular values greater or smaller than α

$$\begin{aligned} Y &= U S V^T \\ &= [U_0 \quad U_1] \begin{bmatrix} S_0 & 0 \\ 0 & S_1 \end{bmatrix} [V_0 \quad V_1]^T \end{aligned}$$

$$D_\alpha(Y) = U_0 (S_0 - \alpha I) V_0^T, \text{ so}$$

$$Y - D_\alpha(Y) =$$

Proximal operator of nuclear norm

Separate SVD of Y into singular values greater or smaller than α

$$\begin{aligned} Y &= U S V^T \\ &= [U_0 \quad U_1] \begin{bmatrix} S_0 & 0 \\ 0 & S_1 \end{bmatrix} [V_0 \quad V_1]^T \end{aligned}$$

$$D_\alpha(Y) = U_0 (S_0 - \alpha I) V_0^T, \text{ so}$$

$$Y - D_\alpha(Y) = \alpha U_0 V_0^T + U_1 S_1 V_1^T$$

Proximal operator of nuclear norm

Separate SVD of Y into singular values greater or smaller than α

$$\begin{aligned} Y &= U S V^T \\ &= [U_0 \quad U_1] \begin{bmatrix} S_0 & 0 \\ 0 & S_1 \end{bmatrix} [V_0 \quad V_1]^T \end{aligned}$$

$$D_\alpha(Y) = U_0 (S_0 - \alpha I) V_0^T, \text{ so}$$

$$\begin{aligned} Y - D_\alpha(Y) &= \alpha U_0 V_0^T + U_1 S_1 V_1^T \\ \frac{1}{\alpha} (Y - D_\alpha(Y)) &= U_0 V_0^T + \frac{1}{\alpha} U_1 S_1 V_1^T \end{aligned}$$

Motivating applications

Convex functions

Optimality conditions

Convex Regularization

Optimization algorithms

Problem

Aim: Minimizing differentiable convex functions

$$\min_{\vec{x} \in \mathbb{R}^n} f(\vec{x})$$

Gradient descent

Intuition: Make local progress in the steepest direction $-\nabla f(\vec{x})$

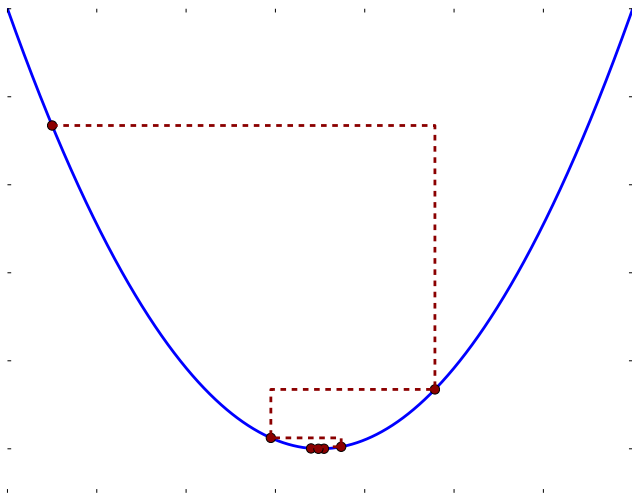
Set the initial point $\vec{x}^{(0)}$ to an arbitrary value

Update by setting

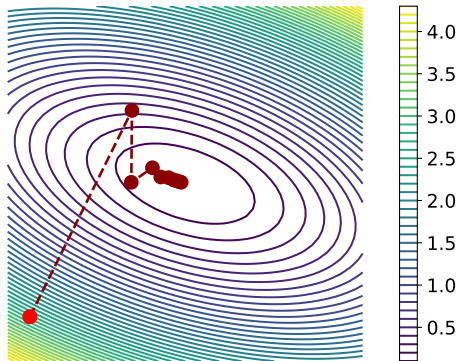
$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f(\vec{x}^{(k)})$$

where $\alpha_k > 0$ is the step size, until a stopping criterion is met

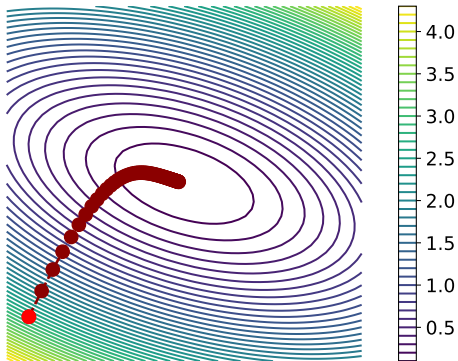
Gradient descent



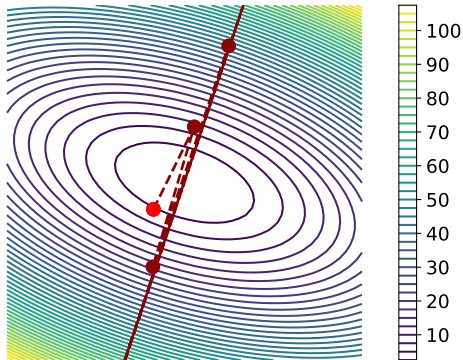
Gradient descent



Small step size



Large step size



Line search

Idea: Find minimum of

$$\begin{aligned}\alpha_k &:= \arg \min_{\alpha} h(\alpha) \\ &= \arg \min_{\alpha \in \mathbb{R}} f\left(\vec{x}^{(k)} - \alpha \nabla f\left(\vec{x}^{(k)}\right)\right)\end{aligned}$$

Problem: Solving 1D convex optimization problem can still be costly

Armijo rule

By convexity of $h := f(\vec{x}^{(k)} - \alpha \nabla f(\vec{x}^{(k)}))$

$$h(\alpha) \geq h(0) + \alpha h'(0)$$

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By differentiability, this is the **only** supporting hyperplane (line)

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For α small enough

$$h(\alpha) \leq h(0) + \frac{\alpha}{2} h'(0)$$

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For α small enough

$$\begin{aligned} h(\alpha) &\leq h(0) + \frac{\alpha}{2} h'(0) \\ &= f(\vec{x}^{(k)}) + \frac{\alpha}{2} \nabla f(\vec{x}^{(k)})^T \left(-\nabla f(\vec{x}^{(k)}) \right) \quad (\text{chain rule}) \end{aligned}$$

Armijo rule

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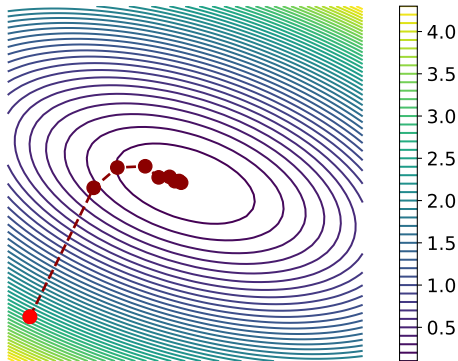
$$\begin{aligned} h(\alpha) &\leq h(0) + \frac{\alpha}{2} h'(0) \\ &= f(\vec{x}^{(k)}) + \frac{\alpha}{2} \nabla f(\vec{x}^{(k)})^T (-\nabla f(\vec{x}^{(k)})) \quad (\text{chain rule}) \\ &= f(\vec{x}^{(k)}) - \frac{\alpha}{2} \|\nabla f(\vec{x}^{(k)})\|_2^2 \end{aligned}$$

Backtracking line search with Armijo rule

Given $\alpha_0 \geq 0$, set $\alpha_k := 0.5^i \alpha_0$ for smallest i such that

$$f\left(\vec{x}^{(k)} - \alpha_k \nabla f\left(\vec{x}^{(k)}\right)\right) \leq f\left(\vec{x}^{(k)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k)}\right) \right\|_2^2$$

Backtracking line search with Armijo rule



Least squares

Let $\vec{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\vec{\beta} \in \mathbb{R}^p$

The gradient of the least-squares cost function

$$f(\vec{\beta}) := \frac{1}{2} \left\| \vec{y} - X\vec{\beta} \right\|_2^2 = \frac{1}{2} \vec{y}^T \vec{y} + \frac{1}{2} \vec{\beta}^T X^T X \vec{\beta} - \vec{y}^T X \vec{\beta}$$

equals

$$\nabla f(\vec{\beta}) = X^T (X\vec{\beta} - \vec{y})$$

Gradient descent for least squares

Gradient descent updates are

$$\vec{\beta}^{(k+1)} = \vec{\beta}^{(k)} + \alpha_k X^T (\vec{y} - X\vec{\beta}^{(k)})$$

Gradient descent for least squares

Gradient descent updates are

$$\begin{aligned}\vec{\beta}^{(k+1)} &= \vec{\beta}^{(k)} + \alpha_k X^T (\vec{y} - X \vec{\beta}^{(k)}) \\ &= \vec{\beta}^{(k)} + \alpha_k \sum_{i=1}^n \left(y^{(i)} - \langle \vec{x}^{(i)}, \vec{\beta}^{(k)} \rangle \right) \vec{x}^{(i)}\end{aligned}$$

Gradient descent for least squares

Let $X^{n \times p}$, $n \geq p$, be full rank with SVD USV^T

The $k + 1$ th iteration of gradient descent with step size $\alpha > 0$ is

$$\begin{aligned}\vec{\beta}^{(k+1)} = & V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\ & + V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \vec{y}\end{aligned}$$

where $\operatorname{diag}_{j=1}^p (d_i)$ is a diagonal matrix with entries $d_1, \dots, d_p$

Proof

$$VV^T = V^T V = I$$

$$\vec{\beta}^{(k+1)} = \left(I - \alpha X^T X \right) \vec{\beta}^{(k)} + \alpha X^T \vec{y}$$

Proof

$$VV^T = V^TV = I$$

$$\begin{aligned}\vec{\beta}^{(k+1)} &= \left(I - \alpha X^T X\right) \vec{\beta}^{(k)} + \alpha X^T \vec{y} \\ &= \left(I - \alpha X^T X\right)^{k+1} \vec{\beta}^{(0)} + \sum_{i=0}^k \left(I - \alpha X^T X\right)^i \alpha X^T \vec{y}\end{aligned}$$

Proof

$$VV^T = V^T V = I$$

$$\begin{aligned}\vec{\beta}^{(k+1)} &= \left(I - \alpha X^T X\right) \vec{\beta}^{(k)} + \alpha X^T \vec{y} \\&= \left(I - \alpha X^T X\right)^{k+1} \vec{\beta}^{(0)} + \sum_{i=0}^k \left(I - \alpha X^T X\right)^i \alpha X^T \vec{y} \\&= \left(VV^T - \alpha VS^2 V^T\right)^{k+1} \vec{\beta}^{(0)} + \alpha \sum_{i=0}^k \left(VV^T - \alpha VS^2 V^T\right)^i VSU^T \vec{y}\end{aligned}$$

Proof

$$VV^T = V^T V = I$$

$$\begin{aligned}\vec{\beta}^{(k+1)} &= \left(I - \alpha X^T X\right) \vec{\beta}^{(k)} + \alpha X^T \vec{y} \\&= \left(I - \alpha X^T X\right)^{k+1} \vec{\beta}^{(0)} + \sum_{i=0}^k \left(I - \alpha X^T X\right)^i \alpha X^T \vec{y} \\&= \left(VV^T - \alpha VS^2 V^T\right)^{k+1} \vec{\beta}^{(0)} + \alpha \sum_{i=0}^k \left(VV^T - \alpha VS^2 V^T\right)^i VSU^T \vec{y} \\&= V \left(I - \alpha S^2\right)^{k+1} V^T \vec{\beta}^{(0)} + \alpha V \sum_{i=0}^k \left(I - \alpha S^2\right)^i V^T VSU^T \vec{y}\end{aligned}$$

Proof

$$\vec{\beta}^{(k+1)} = V (I - \alpha S^2)^{k+1} V^T \vec{\beta}^{(0)} + \alpha V \sum_{i=0}^k (I - \alpha S^2)^i V^T V S U^T \vec{y}$$

Proof

$$\begin{aligned}\vec{\beta}^{(k+1)} &= V (I - \alpha S^2)^{k+1} V^T \vec{\beta}^{(0)} + \alpha V \sum_{i=0}^k (I - \alpha S^2)^i V^T V S U^T \vec{y} \\ &= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\ &\quad + \alpha V \operatorname{diag}_{j=1}^p \left(\sum_{i=0}^k (1 - \alpha s_j^2)^i \right) S U^T \vec{y}\end{aligned}$$

Proof

$$\begin{aligned}\vec{\beta}^{(k+1)} &= V (I - \alpha S^2)^{k+1} V^T \vec{\beta}^{(0)} + \alpha V \sum_{i=0}^k (I - \alpha S^2)^i V^T V S U^T \vec{y} \\&= V \text{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\&\quad + \alpha V \text{diag}_{j=1}^p \left(\sum_{i=0}^k (1 - \alpha s_j^2)^i \right) S U^T \vec{y} \\&= V \text{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\&\quad + \alpha V \text{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\alpha s_j^2} \right) S U^T \vec{y}\end{aligned}$$

Proof

$$\begin{aligned}\vec{\beta}^{(k+1)} &= V (I - \alpha S^2)^{k+1} V^T \vec{\beta}^{(0)} + \alpha V \sum_{i=0}^k (I - \alpha S^2)^i V^T V S U^T \vec{y} \\&= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\&\quad + \alpha V \operatorname{diag}_{j=1}^p \left(\sum_{i=0}^k (1 - \alpha s_j^2)^i \right) S U^T \vec{y} \\&= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\&\quad + \alpha V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\alpha s_j^2} \right) S U^T \vec{y} \\&= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}^{(0)} \\&\quad + \alpha V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\alpha s_j} \right) U^T \vec{y}\end{aligned}$$

Convergence

If $0 < \alpha < 2/s_1^2 \leq 2/s_j^2$ then $|1 - \alpha s_j^2| < 1$

and $\lim_{k \rightarrow \infty} (1 - \alpha s_j^2)^k = 0$

Convergence

If $0 < \alpha < 2/s_1^2 \leq 2/s_j^2$ then $|1 - \alpha s_j^2| < 1$

and $\lim_{k \rightarrow \infty} (1 - \alpha s_j^2)^k = 0$

This implies

$$\begin{aligned}\lim_{k \rightarrow \infty} \vec{\beta}^{(k)} &= \lim_{k \rightarrow \infty} V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) V^T \vec{\beta}^{(0)} \\ &\quad + V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\ &= VS^{-1}U^T \vec{y}\end{aligned}$$

Convergence rate

If $\alpha := 1/s_1^2$ then

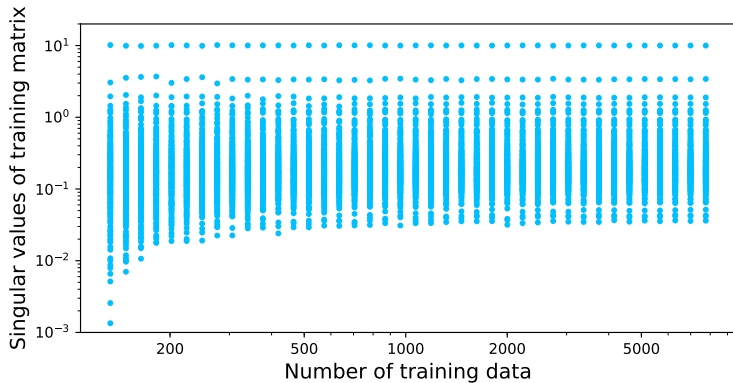
$$\frac{\|\vec{y}_{LS} - \vec{y}^{(k)}\|_2}{\|\vec{y}\|_2} \leq \left(1 - \frac{s_p^2}{s_1^2}\right)^k,$$

s_1 is largest singular value of X and s_p is smallest

Convergence rate is slow if matrix is not well conditioned

Conjugate gradients converges much faster

Temperature prediction via linear regression



Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\ &= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y}\end{aligned}$$

Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\&= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\&= USV^T VS^{-1} U^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y}\end{aligned}$$

Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\&= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\&= USV^T VS^{-1} U^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y} \\&= UU^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y}\end{aligned}$$

Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\&= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\&= USV^T VS^{-1} U^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y} \\&= UU^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y}\end{aligned}$$

Since $\vec{y}_{LS} = UU^T \vec{y}$

$$\left\| \vec{y}_{LS} - \vec{y}^{(k)} \right\|_2 = \left\| U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y} \right\|_2$$

Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\&= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\&= USV^T VS^{-1} U^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y} \\&= UU^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y}\end{aligned}$$

Since $\vec{y}_{LS} = UU^T \vec{y}$

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Proof

$$\begin{aligned}\vec{y}^{(k)} &= X\vec{\beta}^{(k)} \\&= USV^T V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^k}{s_j} \right) U^T \vec{y} \\&= USV^T VS^{-1} U^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y} \\&= UU^T \vec{y} - U \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^k \right) U^T \vec{y}\end{aligned}$$

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Linear regression

Assume additive model for regression problem

$$\vec{y}_{\text{train}} := X_{\text{train}} \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}}$$

Estimate coefficients via gradient descent up to iteration k

Coefficient error equals

$$\begin{aligned} \vec{\beta}_{\text{true}} - \vec{\beta}^{(k+1)} &= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\ &\quad - V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \vec{z}_{\text{train}} \end{aligned}$$

Proof

$$\vec{\beta}^{(k+1)} = V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \left(X_{\text{train}} \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}} \right)$$

Proof

$$\begin{aligned}\vec{\beta}^{(k+1)} &= V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \left(X_{\text{train}} \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}} \right) \\ &= V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \left(USV^T \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}} \right)\end{aligned}$$

Proof

$$\begin{aligned}\vec{\beta}^{(k+1)} &= V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \left(X_{\text{train}} \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}} \right) \\&= V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \left(USV^T \vec{\beta}_{\text{true}} + \vec{z}_{\text{train}} \right) \\&= VS^{-1}U^TUSV^T \vec{\beta}_{\text{true}} - V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\&\quad + V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \vec{z}_{\text{train}} \\&= \vec{\beta}_{\text{true}} - V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\&\quad + V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{s_j} \right) U^T \vec{z}_{\text{train}}\end{aligned}$$

Early stopping

$$\begin{aligned}\vec{\beta}_{\text{true}} - \vec{\beta}^{(k+1)} &= V \text{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\ &\quad - V \text{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\textcolor{red}{s}_j} \right) U^T \vec{z}_{\text{train}}\end{aligned}$$

If sample covariance matrix not close true covariance matrix then
2nd term can produce **noise amplification**

Early stopping

$$\begin{aligned}\vec{\beta}_{\text{true}} - \vec{\beta}^{(k+1)} &= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\ &\quad - V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\color{red}s_j} \right) U^T \vec{z}_{\text{train}}\end{aligned}$$

If sample covariance matrix not close true covariance matrix then
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Selecting small k reduces effect, but increases 1st term

Early stopping

$$\begin{aligned}\vec{\beta}_{\text{true}} - \vec{\beta}^{(k+1)} &= V \operatorname{diag}_{j=1}^p \left((1 - \alpha s_j^2)^{k+1} \right) V^T \vec{\beta}_{\text{true}} \\ &\quad - V \operatorname{diag}_{j=1}^p \left(\frac{1 - (1 - \alpha s_j^2)^{k+1}}{\color{red}s_j} \right) U^T \vec{z}_{\text{train}}\end{aligned}$$

If sample covariance matrix not close true covariance matrix then
2nd term can produce **noise amplification**

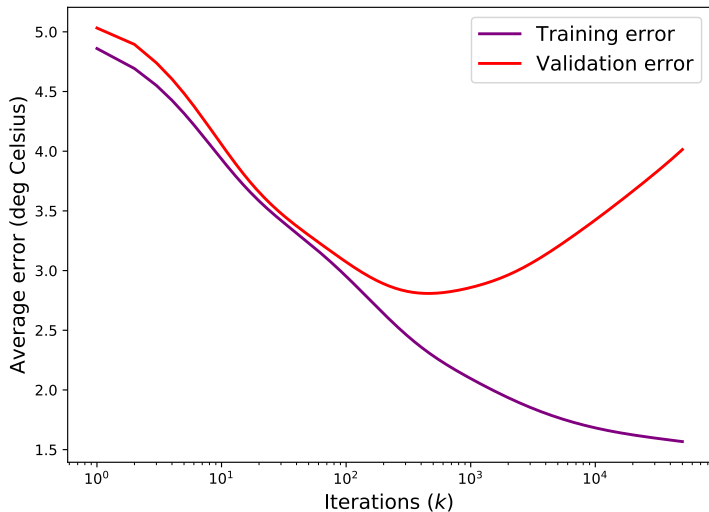
Selecting small k reduces effect, but increases 1st term

Solution: Select best k by minimizing validation error

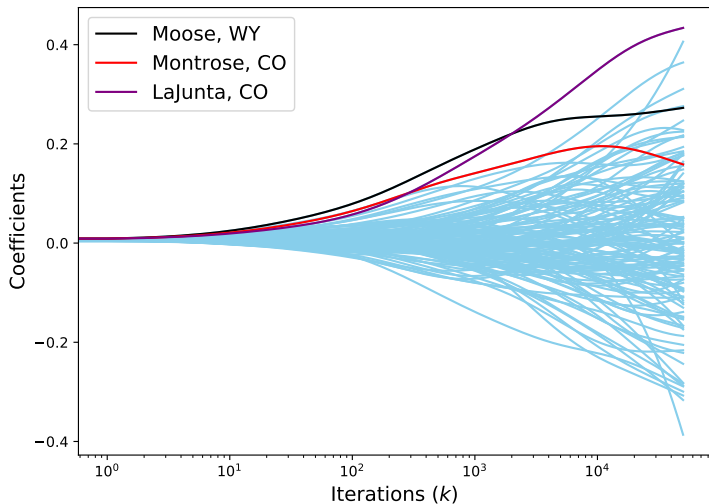
Temperature prediction via linear regression

- ▶ Dataset of hourly temperatures measured at weather stations all over the US
- ▶ Goal: Predict temperature in Yosemite from other temperatures
- ▶ Response: Temperature in Yosemite
- ▶ Features: Temperatures in 133 other stations ($p = 133$) in 2015
- ▶ Test set: 10^3 measurements
- ▶ Additional test set: All measurements from 2016

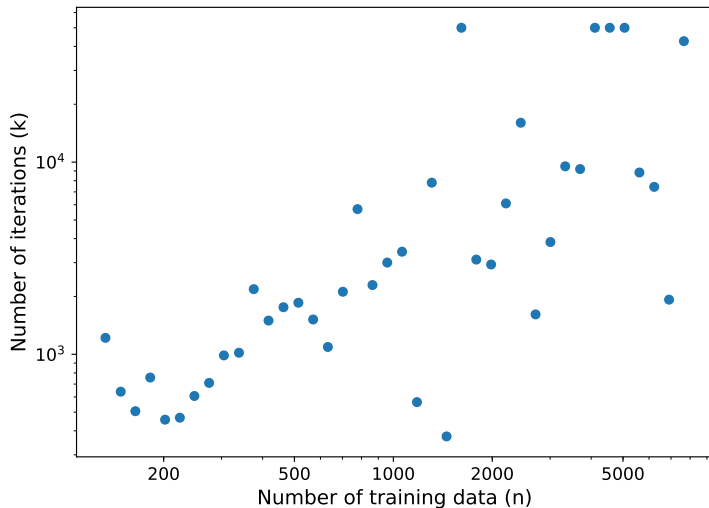
Gradient-descent estimator ($n = 200$)



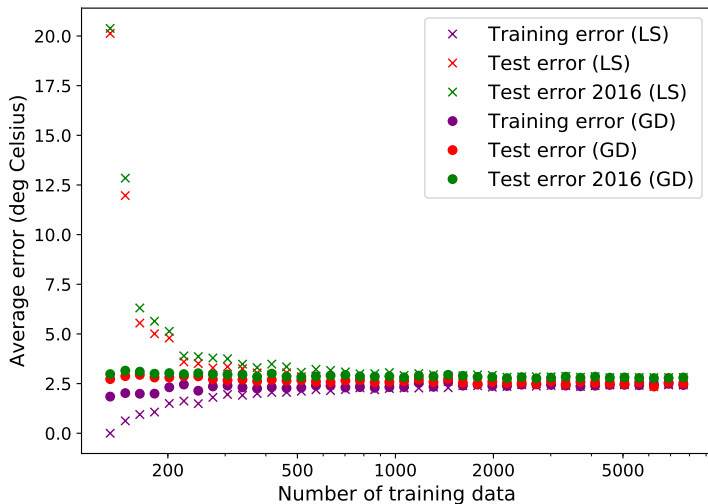
Gradient-descent estimator ($n = 200$)



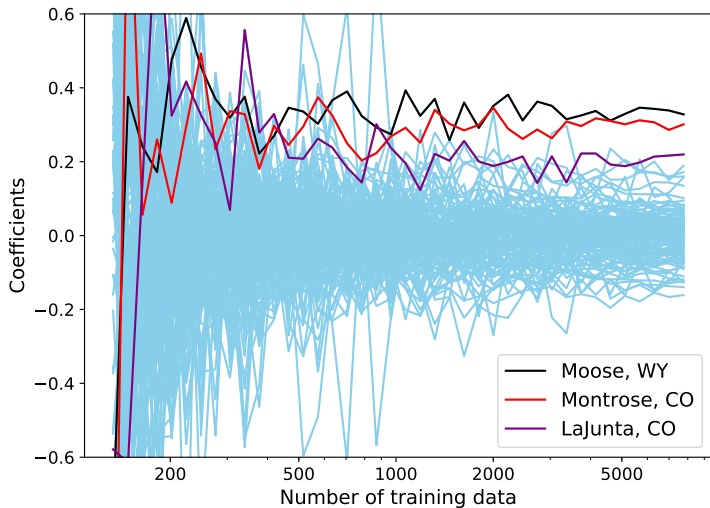
Selected number of iterations



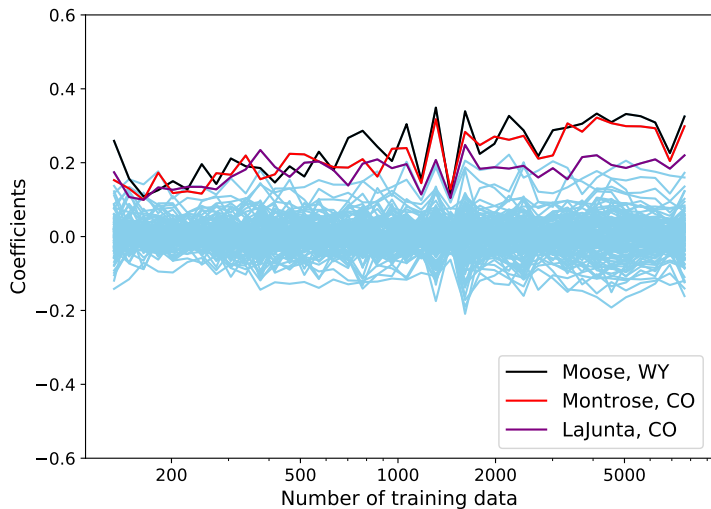
Comparison to least squares



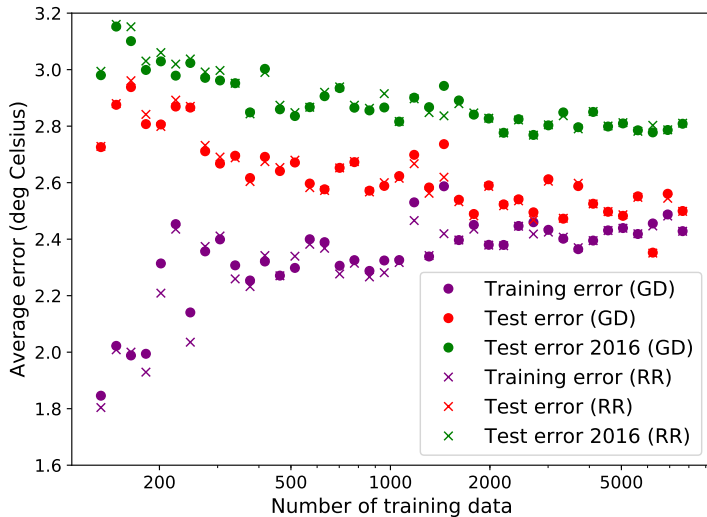
Least-squares coefficients



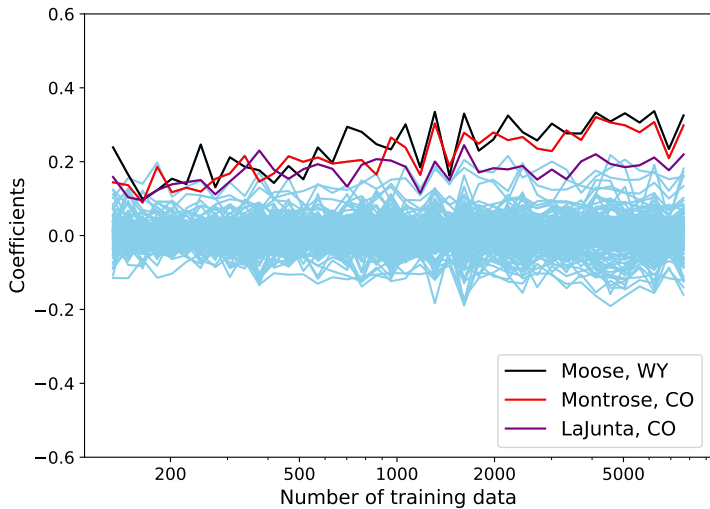
Gradient-descent coefficients



Comparison to ridge regression



Ridge-regression coefficients



Convergence of gradient descent

Functions bounded locally by quadratic with fixed curvature

Satisfied by most reasonable functions

Lipschitz continuity

A function $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is Lipschitz continuous if for any $\vec{x}, \vec{y} \in \mathbb{R}^n$

$$\|g(\vec{y}) - g(\vec{x})\|_2 \leq L \|\vec{y} - \vec{x}\|_2.$$

L is the Lipschitz constant

Lipschitz-continuous gradients

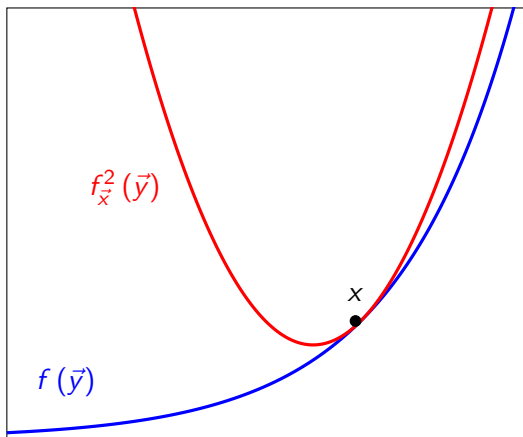
If ∇f is Lipschitz continuous with Lipschitz constant L

$$\|\nabla f(\vec{y}) - \nabla f(\vec{x})\|_2 \leq L \|\vec{y} - \vec{x}\|_2$$

then for any $\vec{x}, \vec{y} \in \mathbb{R}^n$ we have a quadratic upper bound

$$f(\vec{y}) \leq f_{\vec{x}}^2(\vec{y}) := f(\vec{x}) + \nabla f(\vec{x})^T (\vec{y} - \vec{x}) + \frac{L}{2} \|\vec{y} - \vec{x}\|_2^2$$

Quadratic upper bound



Least squares

For any $\vec{\beta}_1, \vec{\beta}_2 \in \mathbb{R}^p$,

$$\left\| \nabla f(\vec{\beta}_2) - \nabla f(\vec{\beta}_1) \right\|_2 = \left\| X^T X (\vec{\beta}_2 - \vec{\beta}_1) \right\|_2 \quad (1)$$

$$\leq s_1^2 \left\| \vec{\beta}_2 - \vec{\beta}_1 \right\|_2 \quad (2)$$

so $L = s_1^2$

Local progress of gradient descent

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f \left(\vec{x}^{(k)} \right)$$

$$f \left(\vec{x}^{(k+1)} \right)$$

Local progress of gradient descent

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f \left(\vec{x}^{(k)} \right)$$

$$\begin{aligned} & f \left(\vec{x}^{(k+1)} \right) \\ & \leq f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(\vec{x}^{(k+1)} - \vec{x}^{(k)} \right) + \frac{L}{2} \left\| \vec{x}^{(k+1)} - \vec{x}^{(k)} \right\|_2^2 \end{aligned}$$

Local progress of gradient descent

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f \left(\vec{x}^{(k)} \right)$$

$$\begin{aligned} & f \left(\vec{x}^{(k+1)} \right) \\ & \leq f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(\vec{x}^{(k+1)} - \vec{x}^{(k)} \right) + \frac{L}{2} \left\| \vec{x}^{(k+1)} - \vec{x}^{(k)} \right\|_2^2 \\ & = f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(-\alpha_k \nabla f \left(\vec{x}^{(k)} \right) \right) + \frac{L}{2} \left\| -\alpha_k \nabla f \left(\vec{x}^{(k)} \right) \right\|_2^2 \end{aligned}$$

Local progress of gradient descent

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f \left(\vec{x}^{(k)} \right)$$

$$\begin{aligned} & f \left(\vec{x}^{(k+1)} \right) \\ & \leq f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(\vec{x}^{(k+1)} - \vec{x}^{(k)} \right) + \frac{L}{2} \left\| \vec{x}^{(k+1)} - \vec{x}^{(k)} \right\|_2^2 \\ & = f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(-\alpha_k \nabla f \left(\vec{x}^{(k)} \right) \right) + \frac{L}{2} \left\| -\alpha_k \nabla f \left(\vec{x}^{(k)} \right) \right\|_2^2 \\ & = f \left(\vec{x}^{(k)} \right) - \alpha_k \left(1 - \frac{\alpha_k L}{2} \right) \left\| \nabla f \left(\vec{x}^{(k)} \right) \right\|_2^2 \end{aligned}$$

Local progress of gradient descent

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k \nabla f(\vec{x}^{(k)})$$

$$\begin{aligned} & f(\vec{x}^{(k+1)}) \\ & \leq f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x}^{(k+1)} - \vec{x}^{(k)}) + \frac{L}{2} \|\vec{x}^{(k+1)} - \vec{x}^{(k)}\|_2^2 \\ & = f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (-\alpha_k \nabla f(\vec{x}^{(k)})) + \frac{L}{2} \|\alpha_k \nabla f(\vec{x}^{(k)})\|_2^2 \\ & = f(\vec{x}^{(k)}) - \alpha_k \left(1 - \frac{\alpha_k L}{2}\right) \|\nabla f(\vec{x}^{(k)})\|_2^2 \end{aligned}$$

$$\text{If } \alpha_k \leq \frac{1}{L}$$

$$f(\vec{x}^{(k+1)}) \leq f(\vec{x}^{(k)}) - \frac{\alpha_k}{2} \|\nabla f(\vec{x}^{(k)})\|_2^2$$

Convergence of gradient descent

- ▶ f is convex
- ▶ ∇f is L -Lipschitz continuous
- ▶ There exists a point $\vec{x}^*$ at which f achieves a finite minimum
- ▶ The step size is set to $\alpha_k := \alpha \leq 1/L$

$$f(\vec{x}^{(k)}) - f(\vec{x}^*) \leq \frac{\|\vec{x}^{(0)} - \vec{x}^*\|_2^2}{2\alpha k}$$

Convergence of gradient descent

$$f\left(\vec{x}^{(k)}\right) \leq f\left(\vec{x}^{(k-1)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

By convexity

$$f\left(\vec{x}^*\right) \geq f\left(\vec{x}^{(k-1)}\right) + \nabla f\left(\vec{x}^{(k-1)}\right)^T \left(\vec{x}^* - \vec{x}^{(k-1)}\right)$$

$$f\left(\vec{x}^{(k)}\right) - f\left(\vec{x}^*\right)$$

Convergence of gradient descent

$$f\left(\vec{x}^{(k)}\right) \leq f\left(\vec{x}^{(k-1)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

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$$f\left(\vec{x}^*\right) \geq f\left(\vec{x}^{(k-1)}\right) + \nabla f\left(\vec{x}^{(k-1)}\right)^T \left(\vec{x}^* - \vec{x}^{(k-1)}\right)$$

$$f\left(\vec{x}^{(k)}\right) - f\left(\vec{x}^*\right)$$

$$\leq f\left(\vec{x}^{(k-1)}\right) - f\left(\vec{x}^*\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

Convergence of gradient descent

$$f\left(\vec{x}^{(k)}\right) \leq f\left(\vec{x}^{(k-1)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

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Convergence of gradient descent

$$f\left(\vec{x}^{(k)}\right) \leq f\left(\vec{x}^{(k-1)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

By convexity

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$$\begin{aligned} & f\left(\vec{x}^{(k)}\right) - f\left(\vec{x}^*\right) \\ & \leq f\left(\vec{x}^{(k-1)}\right) - f\left(\vec{x}^*\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \\ & \leq \nabla f\left(\vec{x}^{(k-1)}\right)^T \left(\vec{x}^{(k-1)} - \vec{x}^*\right) - \frac{\alpha}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \\ & = \frac{1}{2\alpha} \left(\left\| \vec{x}^{(k-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k-1)} - \vec{x}^* - \alpha \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \right) \end{aligned}$$

Convergence of gradient descent

$$f\left(\vec{x}^{(k)}\right) \leq f\left(\vec{x}^{(k-1)}\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2$$

By convexity

$$f\left(\vec{x}^*\right) \geq f\left(\vec{x}^{(k-1)}\right) + \nabla f\left(\vec{x}^{(k-1)}\right)^T \left(\vec{x}^* - \vec{x}^{(k-1)}\right)$$

$$\begin{aligned} & f\left(\vec{x}^{(k)}\right) - f\left(\vec{x}^*\right) \\ & \leq f\left(\vec{x}^{(k-1)}\right) - f\left(\vec{x}^*\right) - \frac{\alpha_k}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \\ & \leq \nabla f\left(\vec{x}^{(k-1)}\right)^T \left(\vec{x}^{(k-1)} - \vec{x}^*\right) - \frac{\alpha}{2} \left\| \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \\ & = \frac{1}{2\alpha} \left(\left\| \vec{x}^{(k-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k-1)} - \vec{x}^* - \alpha \nabla f\left(\vec{x}^{(k-1)}\right) \right\|_2^2 \right) \\ & = \frac{1}{2\alpha} \left(\left\| \vec{x}^{(k-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k)} - \vec{x}^* \right\|_2^2 \right) \end{aligned}$$

Convergence of gradient descent

$$f(\vec{x}^{(k)}) - f(\vec{x}^*)$$

Convergence of gradient descent

$$f(\vec{x}^{(k)}) - f(\vec{x}^*) \leq \frac{1}{k} \sum_{i=1}^k f(\vec{x}^{(i)}) - f(\vec{x}^*)$$

Convergence of gradient descent

$$f(\vec{x}^{(k)}) - f(\vec{x}^*) \leq \frac{1}{k} \sum_{i=1}^k f(\vec{x}^{(i)}) - f(\vec{x}^*) \quad \text{never increases}$$

Convergence of gradient descent

$$\begin{aligned} f(\vec{x}^{(k)}) - f(\vec{x}^*) &\leq \frac{1}{k} \sum_{i=1}^k f(\vec{x}^{(i)}) - f(\vec{x}^*) && \text{never increases} \\ &= \frac{1}{2\alpha k} \sum_{i=1}^k \left\| \vec{x}^{(i-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k)} - \vec{x}^* \right\|_2^2 \end{aligned}$$

Convergence of gradient descent

$$\begin{aligned} f(\vec{x}^{(k)}) - f(\vec{x}^*) &\leq \frac{1}{k} \sum_{i=1}^k f(\vec{x}^{(i)}) - f(\vec{x}^*) && \text{never increases} \\ &= \frac{1}{2\alpha k} \sum_{i=1}^k \left\| \vec{x}^{(i-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k)} - \vec{x}^* \right\|_2^2 \\ &= \frac{1}{2\alpha k} \left(\left\| \vec{x}^{(0)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k)} - \vec{x}^* \right\|_2^2 \right) \end{aligned}$$

Convergence of gradient descent

$$\begin{aligned} f(\vec{x}^{(k)}) - f(\vec{x}^*) &\leq \frac{1}{k} \sum_{i=1}^k f(\vec{x}^{(i)}) - f(\vec{x}^*) && \text{never increases} \\ &= \frac{1}{2\alpha k} \sum_{i=1}^k \left(\left\| \vec{x}^{(i-1)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(i)} - \vec{x}^* \right\|_2^2 \right) \\ &= \frac{1}{2\alpha k} \left(\left\| \vec{x}^{(0)} - \vec{x}^* \right\|_2^2 - \left\| \vec{x}^{(k)} - \vec{x}^* \right\|_2^2 \right) \\ &\leq \frac{\left\| \vec{x}^{(0)} - \vec{x}^* \right\|_2^2}{2\alpha k} \end{aligned}$$

Accelerated gradient descent

- ▶ Gradient descent takes $\mathcal{O}(1/\epsilon)$ to achieve an error of ϵ
- ▶ The optimal rate is $\mathcal{O}(1/\sqrt{\epsilon})$
- ▶ Gradient descent can be **accelerated** by adding a momentum term

Stochastic gradient descent

Cost functions to fit models are often additive

$$f(\vec{x}) = \frac{1}{m} \sum_{i=1}^m f_i(\vec{x}).$$

► Linear regression

$$\sum_{i=1}^n \left(y^{(i)} - \vec{x}^{(i)T} \vec{\beta} \right)^2 = \left\| \vec{y} - X\vec{\beta} \right\|_2^2$$

Stochastic gradient descent

In *big data* regime (very large n), gradient descent is too slow

In some cases, data is acquired sequentially (**online** setting)

Stochastic gradient descent: update solution using a **subset** of the data

Stochastic gradient descent

Set the initial point $\vec{x}^{(0)}$ to an arbitrary value

Update by

1. Choosing a random subset of b indices $\mathcal{B}$ ($b \ll m$ is the batch size)
2. Setting

$$\vec{x}^{(k+1)} := \vec{x}^{(k)} - \alpha_k m \sum_{i \in \mathcal{B}} \nabla f_i(\vec{x}^{(k)})$$

where α_k is the step size

Stochastic gradient descent

For fixed $\vec{x}^{(k)}$ we replace $\nabla f(\vec{x}^{(k)})$ by

$$\sum_{i \in \mathcal{B}} \nabla f_i(\vec{x}^{(k)}) = \sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i(\vec{x}^{(k)})$$

Noisy estimate of ∇f

Stochastic gradient descent

If samples are uniform with replacement, then estimate is aligned with ∇f
on average

$$\mathbb{E} \left(\sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i \left(\vec{x}^{(k)} \right) \right)$$

Stochastic gradient descent

If samples are uniform with replacement, then estimate is aligned with ∇f
on average

$$\mathbb{E} \left(\sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i \left(\vec{x}^{(k)} \right) \right) = \sum_{i=1}^m \mathbb{E} (1_{i \in \mathcal{B}}) \nabla f_i \left(\vec{x}^{(k)} \right)$$

Stochastic gradient descent

If samples are uniform with replacement, then estimate is aligned with ∇f
on average

$$\begin{aligned} \mathbb{E} \left(\sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i \left(\vec{x}^{(k)} \right) \right) &= \sum_{i=1}^m \mathbb{E} (1_{i \in \mathcal{B}}) \nabla f_i \left(\vec{x}^{(k)} \right) \\ &= \sum_{i=1}^m \mathbb{P} (i \in \mathcal{B}) \nabla f_i \left(\vec{x}^{(k)} \right) \end{aligned}$$

Stochastic gradient descent

If samples are uniform with replacement, then estimate is aligned with ∇f
on average

$$\begin{aligned} \mathbb{E} \left(\sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i \left(\vec{x}^{(k)} \right) \right) &= \sum_{i=1}^m \mathbb{E} (1_{i \in \mathcal{B}}) \nabla f_i \left(\vec{x}^{(k)} \right) \\ &= \sum_{i=1}^m \mathbb{P} (i \in \mathcal{B}) \nabla f_i \left(\vec{x}^{(k)} \right) \\ &= \frac{m}{b} \nabla f \left(\vec{x}^{(k)} \right) \end{aligned}$$

Stochastic gradient descent

If samples are uniform with replacement, then estimate is aligned with ∇f
on average

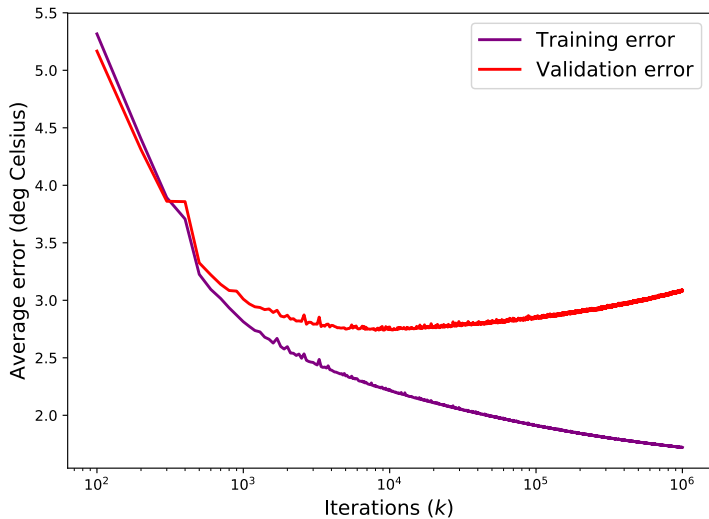
$$\begin{aligned} \mathbb{E} \left(\sum_{i=1}^m 1_{i \in \mathcal{B}} \nabla f_i \left(\vec{x}^{(k)} \right) \right) &= \sum_{i=1}^m \mathbb{E} (1_{i \in \mathcal{B}}) \nabla f_i \left(\vec{x}^{(k)} \right) \\ &= \sum_{i=1}^m \mathbb{P} (i \in \mathcal{B}) \nabla f_i \left(\vec{x}^{(k)} \right) \\ &= \frac{m}{b} \nabla f \left(\vec{x}^{(k)} \right) \end{aligned}$$

Due to variance, α_k needs to be decreasing in k

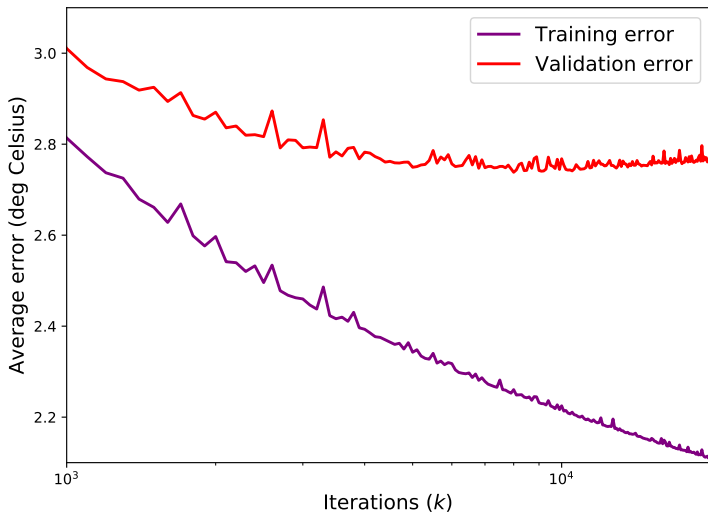
Linear regression

$$\vec{\beta}^{(k+1)} := \vec{\beta}^{(k)} + 2\alpha_k \sum_{i \in \mathcal{B}} \left(\vec{y}^{(i)} - \langle \mathbf{x}^{(i)}, \vec{\beta}^{(k)} \rangle \right) \mathbf{x}^{(i)}$$

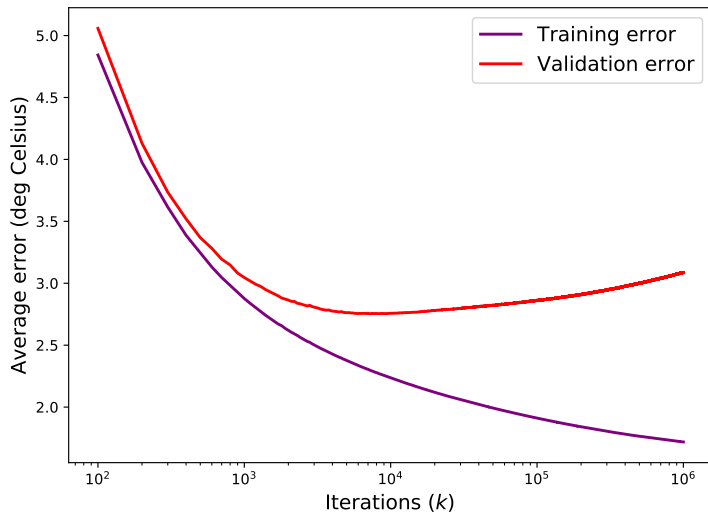
Temperature prediction, batch size = 10



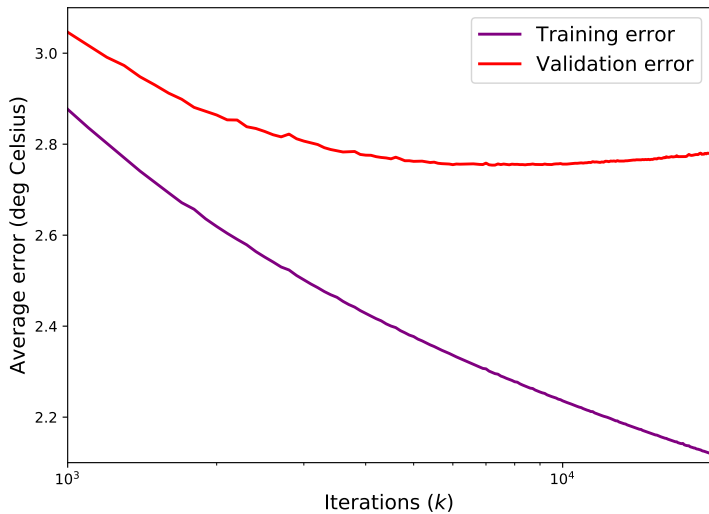
Temperature prediction, batch size = 10



Temperature prediction, batch size = 100



Temperature prediction, batch size = 100



Composite functions

Interesting class of functions for data analysis

$$f(\vec{x}) + h(\vec{x})$$

f convex and differentiable, h convex but not differentiable

Example: Least squares with ℓ_1 -norm or nuclear-norm regularization

Motivation

Aim: Minimize convex differentiable function f

Idea: Iteratively minimize first-order approximation, while staying **close** to current point

$\vec{x}^{(0)}$ = arbitrary initialization

$$\vec{x}^{(k+1)} = \arg \min_{\vec{x}} f\left(\vec{x}^{(k)}\right) + \nabla f\left(\vec{x}^{(k)}\right)^T \left(\vec{x} - \vec{x}^{(k)}\right) + \frac{1}{2\alpha_k} \left\| \vec{x} - \vec{x}^{(k)} \right\|_2^2$$

where α_k is a parameter that determines how close we stay

Motivation

Linear approximation + ℓ_2 term is convex

$$\nabla \left(f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x} - \vec{x}^{(k)}) + \frac{1}{2\alpha_k} \left\| \vec{x} - \vec{x}^{(k)} \right\|_2^2 \right)$$

Motivation

Linear approximation+ ℓ_2 term is convex

$$\begin{aligned} & \nabla \left(f \left(\vec{x}^{(k)} \right) + \nabla f \left(\vec{x}^{(k)} \right)^T \left(\vec{x} - \vec{x}^{(k)} \right) + \frac{1}{2\alpha_k} \left\| \vec{x} - \vec{x}^{(k)} \right\|_2^2 \right) \\ &= \nabla f \left(\vec{x}^{(k)} \right) + \frac{\vec{x} - \vec{x}^{(k)}}{\alpha_k} \end{aligned}$$

Motivation

Linear approximation + ℓ_2 term is convex

$$\begin{aligned} & \nabla \left(f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x} - \vec{x}^{(k)}) + \frac{1}{2\alpha_k} \|\vec{x} - \vec{x}^{(k)}\|_2^2 \right) \\ &= \nabla f(\vec{x}^{(k)}) + \frac{\vec{x} - \vec{x}^{(k)}}{\alpha_k} \end{aligned}$$

Setting the gradient to zero

$$\vec{x}^{(k+1)} = \arg \min_{\vec{x}} f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x} - \vec{x}^{(k)}) + \frac{1}{2\alpha_k} \|\vec{x} - \vec{x}^{(k)}\|_2^2$$

Motivation

Linear approximation + ℓ_2 term is convex

$$\begin{aligned} & \nabla \left(f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x} - \vec{x}^{(k)}) + \frac{1}{2\alpha_k} \|\vec{x} - \vec{x}^{(k)}\|_2^2 \right) \\ &= \nabla f(\vec{x}^{(k)}) + \frac{\vec{x} - \vec{x}^{(k)}}{\alpha_k} \end{aligned}$$

Setting the gradient to zero

$$\begin{aligned} \vec{x}^{(k+1)} &= \arg \min_{\vec{x}} f(\vec{x}^{(k)}) + \nabla f(\vec{x}^{(k)})^T (\vec{x} - \vec{x}^{(k)}) + \frac{1}{2\alpha_k} \|\vec{x} - \vec{x}^{(k)}\|_2^2 \\ &= \vec{x}^{(k)} - \alpha_k \nabla f(\vec{x}^{(k)}) \end{aligned}$$

Proximal gradient method

Idea: Minimize local first-order approximation + h

$$\begin{aligned}\vec{x}^{(k+1)} &= \arg \min_{\vec{x}} f\left(\vec{x}^{(k)}\right) + \nabla f\left(\vec{x}^{(k)}\right)^T \left(\vec{x} - \vec{x}^{(k)}\right) + \frac{1}{2\alpha_k} \left\|\vec{x} - \vec{x}^{(k)}\right\|_2^2 \\ &\quad + h(\vec{x}) \\ &= \arg \min_{\vec{x}} \frac{1}{2} \left\|x - \left(\vec{x}^{(k)} - \alpha_k \nabla f\left(\vec{x}^{(k)}\right)\right)\right\|_2^2 + \alpha_k h(\vec{x}) \\ &= \text{prox}_{\alpha_k h}\left(\vec{x}^{(k)} - \alpha_k \nabla f\left(\vec{x}^{(k)}\right)\right)\end{aligned}$$

Proximal operator:

$$\text{prox}_h(y) := \arg \min_{\vec{x}} h(\vec{x}) + \frac{1}{2} \|y - x\|_2^2$$

Proximal gradient method

Method to solve the optimization problem

$$\text{minimize } f(\vec{x}) + h(\vec{x}),$$

where f is differentiable and prox_h is tractable

Proximal-gradient iteration:

$\vec{x}^{(0)}$ = arbitrary initialization

$$\vec{x}^{(k+1)} = \text{prox}_{\alpha_k h} \left(\vec{x}^{(k)} - \alpha_k \nabla f \left(\vec{x}^{(k)} \right) \right)$$

Interpretation as a fixed-point method

A vector $\vec{x}^*$ is a solution to

$$\text{minimize } f(\vec{x}) + h(\vec{x}),$$

if and only if it is a **fixed point** of the proximal-gradient iteration for any $\alpha > 0$

$$\vec{x}^* = \text{prox}_{\alpha h}(\vec{x}^* - \alpha \nabla f(\vec{x}^*))$$

Proof

$\vec{x}^*$ is the solution to

$$\min_{\vec{x}} \quad \alpha h(\vec{x}) + \frac{1}{2} \|\vec{x}^* - \alpha \nabla f(\vec{x}^*) - \vec{x}\|_2^2$$

if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that

Proof

$\vec{x}^*$ is the solution to

$$\min_{\vec{x}} \quad \alpha h(\vec{x}) + \frac{1}{2} \|\vec{x}^* - \alpha \nabla f(\vec{x}^*) - \vec{x}\|_2^2$$

if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that

$$\alpha \nabla f(\vec{x}^*) + \alpha \vec{g} = \vec{0}$$

Proof

$\vec{x}^*$ is the solution to

$$\min_{\vec{x}} \quad \alpha h(\vec{x}) + \frac{1}{2} \|\vec{x}^* - \alpha \nabla f(\vec{x}^*) - \vec{x}\|_2^2$$

if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that

$$\alpha \nabla f(\vec{x}^*) + \alpha \vec{g} = \vec{0}$$

$\vec{x}^*$ minimizes $f + h$ if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that

Proof

$\vec{x}^*$ is the solution to

$$\min_{\vec{x}} \quad \alpha h(\vec{x}) + \frac{1}{2} \|\vec{x}^* - \alpha \nabla f(\vec{x}^*) - \vec{x}\|_2^2$$

if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that

$$\alpha \nabla f(\vec{x}^*) + \alpha \vec{g} = \vec{0}$$

$\vec{x}^*$ minimizes $f + h$ if and only if there is a subgradient $\vec{g}$ of h at $\vec{x}^*$ such that $\nabla f(\vec{x}^*) + \vec{g} = \vec{0}$

Proximal operator of ℓ_1 norm

The proximal operator of the ℓ_1 norm is the **soft-thresholding operator**

$$\text{prox}_{\alpha \|\cdot\|_1}(y) = \mathcal{S}_\alpha(y)$$

where $\alpha > 0$ and

$$\mathcal{S}_\alpha(y)_i := \begin{cases} y_i - \text{sign}(y_i) \alpha & \text{if } |y_i| \geq \alpha \\ 0 & \text{otherwise} \end{cases}$$

Iterative Shrinkage-Thresholding Algorithm (ISTA)

The proximal gradient method for the problem

$$\text{minimize} \quad \frac{1}{2} \|A\vec{x} - \vec{y}\|_2^2 + \lambda \|\vec{x}\|_1$$

is called ISTA

ISTA iteration:

$\vec{x}^{(0)}$ = arbitrary initialization

$$\vec{x}^{(k+1)} = \mathcal{S}_{\alpha_k \lambda} \left(\vec{x}^{(k)} - \alpha_k A^T (A\vec{x}^{(k)} - \vec{y}) \right)$$

Proximal operator of nuclear norm

The solution X to

$$\min_{X \in \mathbb{R}^{m \times n}} \frac{1}{2} \|Y - X\|_F^2 + \tau \|X\|_*$$

is obtained by **soft-thresholding** the SVD of Y

$$X_{\text{prox}} = \mathcal{D}_\tau(Y)$$

$$\mathcal{D}_\tau(M) := U \mathcal{S}_\tau(S) V^T \quad \text{where } M = U S V^T$$

$$\mathcal{S}_\tau(S)_{ii} := \begin{cases} S_{ii} - \tau & \text{if } S_{ii} > \tau \\ 0 & \text{otherwise} \end{cases}$$

Proximal gradient method

Proximal gradient method for the problem

$$\min_{X \in \mathbb{R}^{m \times n}} ||X_{\Omega} - \vec{y}||_2^2 + \lambda ||X||_*$$

$X^{(0)}$ = arbitrary initialization

$$M^{(k)} = X^{(k)} - \alpha_k \left(X_{\Omega}^{(k)} - \vec{y} \right)$$

$$X^{(k+1)} = \mathcal{D}_{\alpha_k \lambda} \left(M^{(k)} \right)$$

Results

