Optimization in Machine Learning

Mathematical Concepts Quadratic forms II

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Learning goals

- Geometry of quadratic forms
- Spectrum of Hessian

PROPERTIES OF QUADRATIC FUNCTIONS Recall: Quadratic form *q*

- \bullet Univariate: $q(x) = ax^2 + bx + c$
- Multivariate: $q(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$

General observation: If $q \geq 0$ ($q \leq 0$), q is convex (concave)

Univariate function: Second derivative is $q''(x) = 2a$

- $q''(x) \stackrel{(>)}{\geq} 0$: *q* (strictly) convex. $q''(x) \stackrel{(<)}{\leq} 0$: *q* (strictly) concave.
- High (low) absolute values of $q''(x)$: high (low) curvature

Multivariate function: Second derivative is **H** = 2**A**

- Convexity/concavity of *q* depend on eigenvalues of **H**
- Let us look at an example of the form $q(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$

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GEOMETRY OF QUADRATIC FUNCTIONS

Example:
$$
A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \implies H = 2A = \begin{pmatrix} 4 & -2 \\ -2 & 4 \end{pmatrix}
$$

Since **H** symmetric, eigendecomposition $H = V \Lambda V^T$ with

$$
\mathbf{V} = \begin{pmatrix} | & | \\ v_{\text{max}} & v_{\text{min}} \\ | & | \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \text{ orthogonal}
$$

$$
\text{ and } \Lambda = \begin{pmatrix} \lambda_{max} & 0 \\ 0 & \lambda_{min} \end{pmatrix} = \begin{pmatrix} 6 & 0 \\ 0 & 2 \end{pmatrix}.
$$

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$$

GEOMETRY OF QUADRATIC FUNCTIONS / 2

*v*max (*v*min) direction of highest (lowest) curvature **Proof:** With $v = V^T x$:

$$
\mathbf{x}^T \mathbf{H} \mathbf{x} = \mathbf{x}^T \mathbf{V} \Lambda \mathbf{V}^T \mathbf{x} = \mathbf{v}^T \Lambda \mathbf{v} = \sum_{i=1}^d \lambda_i v_i^2 \le \lambda_{\text{max}} \sum_{i=1}^d v_i^2 = \lambda_{\text{max}} ||\mathbf{v}||^2
$$

 $\textsf{Since } \|\textbf{v}\| = \|\textbf{x}\|$ (**V** orthogonal): max $_{\|\textbf{x}\|=1}$ $\textbf{x}^{\mathsf{T}}\textbf{H}\textbf{x} \leq \lambda_{\textsf{max}}$ Additional: $\mathbf{v}_{\text{max}}^T \mathbf{H} \mathbf{v}_{\text{max}} = \mathbf{e}_1^T \mathbf{\Lambda} \mathbf{e}_1 = \lambda_{\text{max}}$ Analogous: $\min_{\|\mathbf{x}\|=1} \mathbf{x}^{\mathsf{T}}\mathsf{H}\mathbf{x} \geq \lambda_{\textsf{min}}$ and $\mathbf{v}_{\textsf{min}}{}^{\mathsf{T}}\mathsf{H}\mathbf{v}_{\textsf{min}} = \lambda_{\textsf{min}}$

Contour lines of any quadratic form are ellipses (with eigenvectors of A as principal axes, principal axis theorem) Look at $q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x} + \boldsymbol{b}^T \mathbf{x} + c$ Now use $y = x - w = x + \frac{1}{2}A^{-1}b$ This already gives us the general form of an ellipse: $\mathbf{y}^T A \mathbf{y} = (\mathbf{x} - \mathbf{w})^T \mathbf{A} (\mathbf{x} - \mathbf{w}) = q(\mathbf{x}) + const$ If we use $\mathbf{z} = \mathbf{V}^T \mathbf{y}$ we obtain it in standard form $\sum_{i=1}^{n} \lambda_i z_i^2 = \mathbf{z}^T \mathbf{\Lambda} \mathbf{z} = y^T \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T y = \mathbf{y}^T \mathbf{A} \mathbf{y} = q(\mathbf{x}) + \text{const}$

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GEOMETRY OF QUADRATIC FUNCTIONS / 3

Recall: **Second order condition for optimality** is **sufficient**.

We skipped the **proof** at first, but can now catch up on it. If $H(\mathbf{x}^*) \succ 0$ at stationary point \mathbf{x}^* , then \mathbf{x}^* is local minimum (\prec for maximum).

Proof: Let $\lambda_{\text{min}} > 0$ denote the smallest eigenvalue of $H(\mathbf{x}^*)$. Then:

$$
f(\mathbf{x}) = f(\mathbf{x}^*) + \underbrace{\nabla f(\mathbf{x}^*)}_{=0}^T(\mathbf{x} - \mathbf{x}^*) + \frac{1}{2} \underbrace{(\mathbf{x} - \mathbf{x}^*)^T H(\mathbf{x}^*) (\mathbf{x} - \mathbf{x}^*)}_{\geq \lambda_{\text{min}} ||\mathbf{x} - \mathbf{x}^*||^2 \text{ (see above)}} + \underbrace{B_2(\mathbf{x}, \mathbf{x}^*)}_{=o(||\mathbf{x} - \mathbf{x}^*||^2)}.
$$

Choose $\epsilon > 0$ s.t. $|R_2(\mathbf{x}, \mathbf{x}^*)| < \frac{1}{2}\lambda_{\text{min}} \|\mathbf{x} - \mathbf{x}^*\|^2$ for each $\mathbf{x} \neq \mathbf{x}^*$ with $\|\mathbf{x} - \mathbf{x}^*\| < \epsilon$. Then:

$$
f(\mathbf{x}) \geq f(\mathbf{x}^*) + \underbrace{\frac{1}{2}\lambda_{\min}\|\mathbf{x} - \mathbf{x}^*\|^2 + B_2(\mathbf{x}, \mathbf{x}^*)}_{>0} > f(\mathbf{x}^*) \quad \text{for each } \mathbf{x} \neq \mathbf{x}^* \text{ with } \|\mathbf{x} - \mathbf{x}^*\| < \epsilon.
$$

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GEOMETRY OF QUADRATIC FUNCTIONS / 4

If spectrum of \bf{A} is known, also that of $\bf{H} = 2\bf{A}$ is known.

- If **all** eigenvalues of **H** \geq 0 (⇔ **H** \geq 0):
	- *q* (strictly) convex,
	- there is a (unique) global minimum.
- If **all** eigenvalues of **H** \leq 0 (\Leftrightarrow **H** \leq 0):
	- *q* (strictly) concave,
	- there is a (unique) global maximum.
- If **H** has both positive and negative eigenvalues (⇔ **H** indefinite):
	- *q* neither convex nor concave,
	- there is a saddle point.

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CONDITION AND CURVATURE

Condition of **H** = 2**A** is given by $\kappa(H) = \kappa(\mathbf{A}) = |\lambda_{\text{max}}|/|\lambda_{\text{min}}|$.

High condition means:

- \bullet $|\lambda_{\text{max}}| \gg |\lambda_{\text{min}}|$
- **Curvature along** v_{max} \gg **curvature along** v_{min}
- **Problem** for optimization algorithms like **gradient descent** (later)

Left: Excellent condition. **Middle:** Good condition. **Right:** Bad condition.

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APPROXIMATION OF SMOOTH FUNCTIONS

Any function $f\in \mathcal{C}^2$ can be locally approximated by a quadratic function via second order Taylor approximation:

$$
f(\mathbf{x}) \approx f(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}})^T(\mathbf{x} - \tilde{\mathbf{x}}) + \frac{1}{2}(\mathbf{x} - \tilde{\mathbf{x}})^T \nabla^2 f(\tilde{\mathbf{x}})(\mathbf{x} - \tilde{\mathbf{x}})
$$

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f and its second order approximation is shown by the dark and bright grid, respectively. (Source: <daniloroccatano.blog>)

 \implies Hessians provide information about **local** geometry of a function.