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*

• 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 $q \ge 0$ ($q \le 0$), 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 = 2A

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

• Since **H** symmetric, eigendecomposition $\mathbf{H} = \mathbf{V} \wedge \mathbf{V}^{T}$ with

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

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

- \mathbf{v}_{\max} (\mathbf{v}_{\min}) direction of highest (lowest) curvature Proof: With $\mathbf{v} = \mathbf{V}^T \mathbf{x}$: $\mathbf{x}^T \mathbf{H} \mathbf{x} = \mathbf{x}^T \mathbf{V} \wedge \mathbf{V}^T \mathbf{x} = \mathbf{v}^T \wedge \mathbf{v} = \sum_{i=1}^d \lambda_i v_i^2 \le \lambda_{\max} \sum_{i=1}^d v_i^2 = \lambda_{\max} ||\mathbf{v}||^2$ Since $||\mathbf{v}|| = ||\mathbf{x}||$ (V orthogonal): $\max_{||\mathbf{x}||=1} \mathbf{x}^T \mathbf{H} \mathbf{x} \le \lambda_{\max}$ Additional: $\mathbf{v}_{\max}^T \mathbf{H} \mathbf{v}_{\max} = \mathbf{e}_1^T \wedge \mathbf{e}_1 = \lambda_{\max}$ Analogous: $\min_{||\mathbf{x}||=1} \mathbf{x}^T \mathbf{H} \mathbf{x} \ge \lambda_{\min}$ and $\mathbf{v}_{\min}^T \mathbf{H} \mathbf{v}_{\min} = \lambda_{\min}$
- Contour lines of any quadratic form are ellipses (with eigenvectors of A as principal axes, principal axis theorem) Look at q(x) = x^TAx + b^Tx + c Now use y = x - w = x + ½A⁻¹b This already gives us the general form of an ellipse: y^TAy = (x - w)^TA(x - w) = q(x) + const If we use z = V^Ty we obtain it in standard form ∑ⁿ_{i=1} λ_iz²_i = z^TΛz = y^TVΛV^Ty = y^TAy = q(x) + const

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

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \underbrace{\nabla f(\mathbf{x}^*)}_{=0}^T (\mathbf{x} - \mathbf{x}^*) + \frac{1}{2} \underbrace{(\mathbf{x} - \mathbf{x}^*)^T H(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*)}_{\geq \lambda_{\min} \|\|\mathbf{x} - \mathbf{x}^*\|^2 \text{ (see above)}} + \underbrace{H_2(\mathbf{x}, \mathbf{x}^*)}_{=o(\|\|\mathbf{x} - \mathbf{x}^*\|^2)}$$

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

$$f(\mathbf{x}) \ge f(\mathbf{x}^*) + \underbrace{\frac{1}{2} \lambda_{\min} \|\mathbf{x} - \mathbf{x}^*\|^2}_{>0} + R_2(\mathbf{x}, \mathbf{x}^*)}_{>0} > f(\mathbf{x}^*) \quad \text{for each } \mathbf{x} \neq \mathbf{x}^* \text{ with } \|\mathbf{x} - \mathbf{x}^*\| < \epsilon.$$

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GEOMETRY OF QUADRATIC FUNCTIONS / 4

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

- If all eigenvalues of $\mathbf{H} \stackrel{(>)}{\geq} \mathbf{0} \iff \mathbf{H} \stackrel{(\succ)}{\succ} \mathbf{0}$:
 - q (strictly) convex,
 - there is a (unique) global minimum.
- If all eigenvalues of $\mathbf{H} \stackrel{(<)}{\leq} \mathbf{0} \iff \mathbf{H} \stackrel{(\prec)}{\preccurlyeq} \mathbf{0}$:
 - q (strictly) concave,
 - there is a (unique) global maximum.
- $\bullet~$ If H has both positive and negative eigenvalues (\Leftrightarrow H indefinite):
 - q neither convex nor concave,
 - there is a saddle point.



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CONDITION AND CURVATURE

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

High condition means:

- $\bullet \ |\lambda_{\max}| \gg |\lambda_{\min}|$
- 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.

Optimization in Machine Learning - 6 / 7

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APPROXIMATION OF SMOOTH FUNCTIONS

Any function $f \in C^2$ 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.