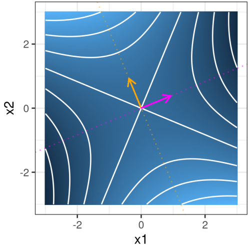
Optimization in Machine Learning

Mathematical Concepts
Quadratic forms II



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: $q(\mathbf{x}) = \mathbf{x}^T\mathbf{A}\mathbf{x} + \boldsymbol{b}^T\mathbf{x} + c$

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

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

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

Multivariate function: Second derivative is $\mathbf{H} = 2\mathbf{A}$

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

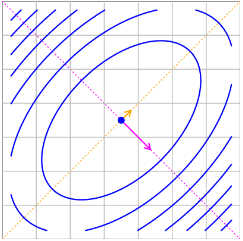
GEOMETRY OF QUADRATIC FUNCTIONS

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 $\mathbf{H}$ symmetric, eigendecomposition $\mathbf{H} = \mathbf{V}\Lambda\mathbf{V}^T$ with

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

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



GEOMETRY OF QUADRATIC FUNCTIONS / 2

- $\boldsymbol{v}_{\max}$ ($\boldsymbol{v}_{\min}$) direction of highest (lowest) curvature

  Proof: With $\boldsymbol{v} = \mathbf{V}^T\mathbf{x}$:

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

  Since $\|\boldsymbol{v}\| = \|\mathbf{x}\|$ ($\mathbf{V}$ orthogonal): $\max_{\|\mathbf{x}\|=1}\mathbf{x}^T\mathbf{H}\mathbf{x} \leq \lambda_{\max}$
  Additional: $\boldsymbol{v}_{\max}{}^T\mathbf{H}\boldsymbol{v}_{\max} = \mathbf{e}_1^T\Lambda\mathbf{e}_1 = \lambda_{\max}$

  Analogous: $\min_{\|\mathbf{x}\|=1}\mathbf{x}^T\mathbf{H}\mathbf{x} \geq \lambda_{\min}$ and $\boldsymbol{v}_{\min}{}^T\mathbf{H}\boldsymbol{v}_{\min} = \lambda_{\min}$

- Contour lines of any quadratic form are ellipses
  (with eigenvectors of A as principal axes, principal axis theorem)

  Look at $q(\mathbf{x}) = \mathbf{x}^T\boldsymbol{A}\mathbf{x} + \boldsymbol{b}^T\mathbf{x} + c$
  Now use $\boldsymbol{y} = \mathbf{x} - \boldsymbol{w} = \mathbf{x} + \frac{1}{2}\boldsymbol{A}^{-1}\boldsymbol{b}$
  This already gives us the general form of an ellipse:
  $\boldsymbol{y}^T\boldsymbol{A}\boldsymbol{y} = (\mathbf{x} - \boldsymbol{w})^T\boldsymbol{A}(\mathbf{x} - \boldsymbol{w}) = q(\mathbf{x}) + const$
  If we use $\boldsymbol{z} = \boldsymbol{V}^T y$ we obtain it in standard form
  $\sum_{i=1}^{n}\lambda_i z_i^2 = \boldsymbol{z}^T\boldsymbol{\Lambda}\boldsymbol{z} = y^T\boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T y = \boldsymbol{y}^T\boldsymbol{A}\boldsymbol{y} = q(\mathbf{x}) + const$

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

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \underbrace{\nabla f(\mathbf{x}^*)}_{=0}{}^T(\mathbf{x} - \mathbf{x}^*) + \frac{1}{2}\underbrace{(\mathbf{x} - \mathbf{x}^*)^T H(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*)}_{\geq \lambda_{\text{min}} \|\mathbf{x} - \mathbf{x}^*\|^2 \text{ (see above)}} + \underbrace{R_2(\mathbf{x}, \mathbf{x}^*)}_{= o(\|\mathbf{x} - \mathbf{x}^*\|^2)} .$$

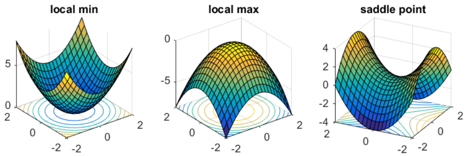
Choose $\epsilon > 0$ s.t. $|R_2(\mathbf{x}, \mathbf{x}^*)| < \frac{1}{2}\lambda_{\text{min}}\|\mathbf{x} - \mathbf{x}^*\|^2$ for each $\mathbf{x} \neq \mathbf{x}^*$ with $\|\mathbf{x} - \mathbf{x}^*\| < \epsilon$.
Then:

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

GEOMETRY OF QUADRATIC FUNCTIONS / 4

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

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

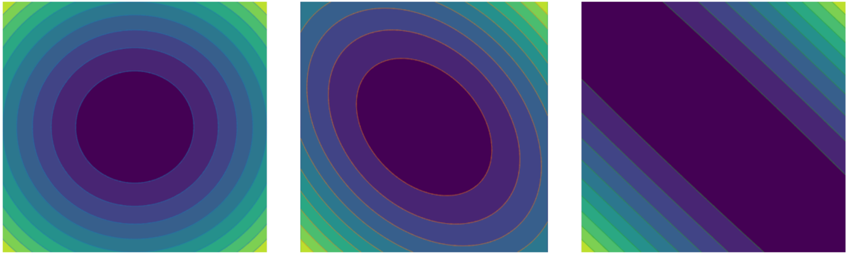


CONDITION AND CURVATURE

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

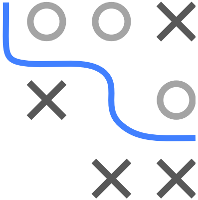
High condition means:

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



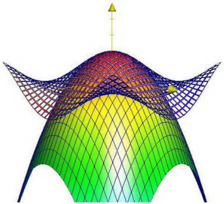
Left: Excellent condition. **Middle:** Good condition. **Right:** Bad condition.

APPROXIMATION OF SMOOTH FUNCTIONS



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

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



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

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