Newton-Raphson step. Quadratic expansion

$$E_* \approx E + \Delta\mathbf{x}_*^{\mathrm{t}}\mathbf{g} + \tfrac{1}{2}\Delta\mathbf{x}_*^{\mathrm{t}}\mathbf{H}\Delta\mathbf{x}_* \qquad \mathbf{x}_* \equiv \mathbf{x} + \Delta\mathbf{x}_*$$

Linear gradient expansion

$$\mathbf{g}_* = \mathbf{g} + \mathbf{H}\Delta\mathbf{x}_*$$

Setting the gradient at the next point to zero gives the Newton-Raphson step

$$\mathbf{g}_* \overset{!}{=} \mathbf{0} \implies \Delta\mathbf{x}_* = -\mathbf{H}^{-1}\mathbf{g}$$

For a perfectly quadratic surface, the Hessian is constant and the Newton-Raphson step takes us directly to the stationary point. On a surface with cubic and higher-order terms, this step can be repeated iteratively until we are close enough to the stationary point that the region separating us from it is approximately quadratic.

Quasi-Newton condition. For points $\mathbf{x}$ and $\mathbf{x}_0$ sharing a locally quadratic region with each other, the change in the gradient between them is described by the following.

$$\mathbf{H}\Delta\mathbf{x} \approx \mathbf{H}_0\Delta\mathbf{x} \approx \Delta\mathbf{g} \qquad \begin{array}{l} \Delta\mathbf{x} \equiv \mathbf{x} - \mathbf{x}_0 \\ \Delta\mathbf{g} \equiv \mathbf{g} - \mathbf{g}_0 \end{array}$$

This can be used to determine an approximation $\tilde{\mathbf{H}} \approx \mathbf{H}$ to the Hessian at $\mathbf{x}$ using the Hessian at the other point. Namely, we require the approximation to satisfy

$$\tilde{\mathbf{H}}\Delta\mathbf{x} \overset{!}{=} \Delta\mathbf{g} \qquad \tilde{\mathbf{H}} = \mathbf{H}_0 + \Delta\tilde{\mathbf{H}}$$

which is known as the *quasi-Newton condition*. If the dimension is d, then we have d linear equations and d^2 elements in the correction matrix, so this equation is underdetermined. One simple choice is a rank-1 approximation

$$\Delta\tilde{\mathbf{H}} = \eta\,\mathbf{e}\mathbf{e}^{\mathrm{t}}$$