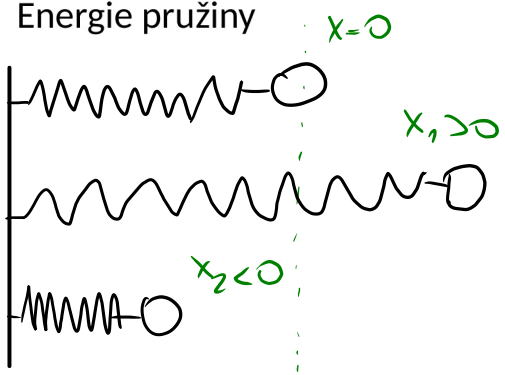
# Funkce více proměnných

Tomáš Raček

# Potenciální energie vazby

optimální délka $d_0$

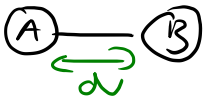
Energie pružiny



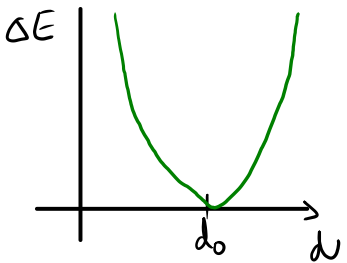

$E = \frac{1}{2} k x^2$

↑ tuhost pružiny

Energie vazby



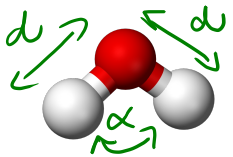

$\Delta E(d) = k \cdot (d - d_0)^2$



# Molekula vody I

Potenciální energie závisí na:

- délka O-H vazby
- velikost úhlu H-O-H




$\alpha_0$ = optimální velikost úhlu H-O-H

$$\Delta E(\alpha) = k \cdot (\alpha - \alpha_0)^2$$

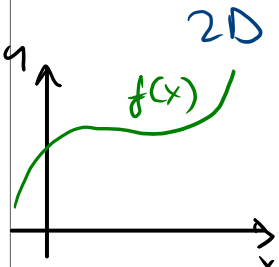
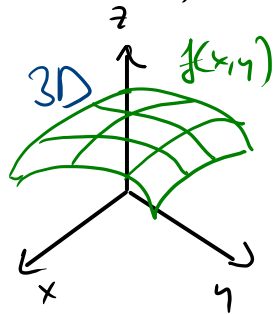
DOHROMADY:

$$\Delta E(d, \alpha) = k_1 \cdot (d - d_0)^2 + k_2 \cdot (\alpha - \alpha_0)^2$$

↑ celková $\Delta E$

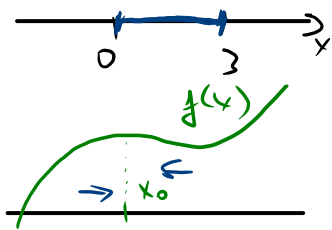
? potřeba zjistit z experimentu

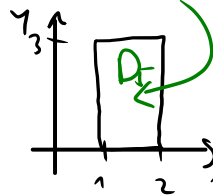
# Funkce jedné, dvou a více proměnných

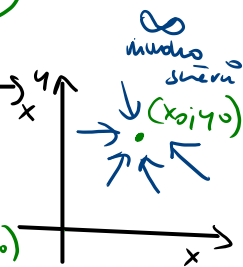
| | 1 proměnná | 2 proměnné | N proměnných |
|---|---|---|---|
| Předpis | $y = f(x)$ | $z = f(x, y)$ | $y = f(x_1, x_2, \dots, x_N)$ |
| Příklad | $y = x^3 + \sin x$<br>$S = \pi r^2$ | $z = x^2 + \sqrt{y}$<br>$\Delta \in (a, \alpha) = \dots$ | $y = x_1 \cdot x_2 + \sin x_3 + x_4$ |
| Graf |  |  | $(N+1)D$<br>?<br>. |

# Funkce jedné a dvou proměnných – příklady vlastností

| | 1 proměnná | 2 proměnné |
|---|---|---|
| Definiční obor | $D_1 = \mathbb{R}$<br>$D_2 = [0;3]$<br>$D_3 = (-\infty; 1)$ | $D_4 = \mathbb{R} \times \mathbb{R}$<br>$D_5 = [1;2] \times [0;3]$ |
| Limity | $\lim_{x \to x_0} f(x)$ | $\lim_{(x,y) \to (x_0,y_0)}$ |



# Tabulky funkčních hodnot

$g(x,y) = x \cdot y$

## 1 proměnná

| $x$ | $-2$ | $-1$ | $0$ | $1$ | $2$ |
|---|---|---|---|---|---|
| $f(x)$ | 5 | 2 | 1 | 2 | 5 |

$f(x) = x^2 + 1$

## 2 proměnné

| $x/y$ | $-2$ | $-1$ | $0$ | $1$ | $2$ |
|---|---|---|---|---|---|
| $-2$ | | | | | |
| $-1$ | | 1 | | | |
| $0$ | | | | | |
| $1$ | | | | | |
| $2$ | | | | | |

$g(0,1)$

# Molekula vody II

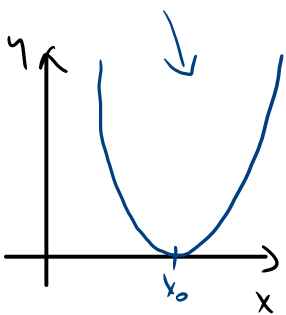
| H-O-H (Å) / O-H (°) | 0.900 | 0.905 | 0.910 | 0.915 | 0.920 | 0.925 | 0.930 | 0.935 | 0.940 | 0.945 | 0.950 | 0.955 | 0.960 | 0.965 | 0.970 | 0.975 | 0.980 | 0.985 | 0.990 | 0.995 | 1.000 | 1.005 | 1.010 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 93.0 | 7.911 | 6.995 | 6.168 | 5.424 | 4.764 | 4.182 | 3.678 | 3.247 | 2.889 | 2.600 | 2.377 | 2.220 | 2.125 | 2.091 | 2.115 | 2.195 | 2.330 | 2.517 | 2.755 | 3.043 | 3.377 | 3.757 | 4.181 |
| 93.5 | 7.671 | 6.760 | 5.936 | 5.198 | 4.542 | 3.967 | 3.465 | 3.039 | 2.684 | 2.400 | 2.182 | 2.028 | 1.938 | 1.908 | 1.936 | 2.020 | 2.159 | 2.350 | 2.592 | 2.883 | 3.222 | 3.605 | 4.032 |
| 94.0 | 7.440 | 6.534 | 5.715 | 4.981 | 4.329 | 3.757 | 3.261 | 2.839 | 2.489 | 2.209 | 1.995 | 1.846 | 1.760 | 1.733 | 1.766 | 1.854 | 1.997 | 2.192 | 2.438 | 2.733 | 3.075 | 3.465 | 3.894 |
| 94.5 | 7.219 | 6.317 | 5.503 | 4.773 | 4.126 | 3.558 | 3.066 | 2.649 | 2.304 | 2.027 | 1.818 | 1.673 | 1.590 | 1.565 | 1.604 | 1.697 | 1.844 | 2.043 | 2.292 | 2.591 | 2.937 | 3.329 | 3.763 |
| 95.0 | 7.008 | 6.110 | 5.300 | 4.575 | 3.932 | 3.368 | 2.881 | 2.468 | 2.127 | 1.855 | 1.649 | 1.508 | 1.430 | 1.412 | 1.452 | 1.548 | 1.699 | 1.902 | 2.156 | 2.458 | 2.807 | 3.202 | 3.641 |
| 95.5 | 6.805 | 5.912 | 5.107 | 4.386 | 3.748 | 3.188 | 2.705 | 2.296 | 1.959 | 1.691 | 1.490 | 1.353 | 1.279 | 1.264 | 1.308 | 1.409 | 1.563 | 1.770 | 2.027 | 2.333 | 2.686 | 3.085 | 3.527 |
| 96.0 | 6.613 | 5.724 | 4.923 | 4.207 | 3.573 | 3.017 | 2.538 | 2.134 | 1.801 | 1.537 | 1.339 | 1.206 | 1.136 | 1.126 | 1.174 | 1.278 | 1.436 | 1.646 | 1.907 | 2.217 | 2.574 | 2.976 | 3.422 |
| 96.5 | 6.429 | 5.545 | 4.748 | 4.036 | 3.406 | 2.855 | 2.381 | 1.985 | 1.651 | 1.391 | 1.198 | 1.069 | 1.002 | 0.996 | 1.048 | 1.155 | 1.317 | 1.531 | 1.795 | 2.109 | 2.470 | 2.875 | 3.324 |
| 97.0 | 6.255 | 5.375 | 4.583 | 3.875 | 3.249 | 2.702 | 2.232 | 1.835 | 1.510 | 1.254 | 1.065 | 0.940 | 0.877 | 0.875 | 0.930 | 1.042 | 1.207 | 1.425 | 1.695 | 2.010 | 2.374 | 2.783 | 3.236 |
| 97.5 | 6.091 | 5.215 | 4.426 | 3.723 | 3.101 | 2.558 | 2.092 | 1.699 | 1.378 | 1.126 | 0.941 | 0.820 | 0.761 | 0.762 | 0.821 | 0.936 | 1.105 | 1.327 | 1.599 | 1.919 | 2.286 | 2.699 | 3.155 |
| 98.0 | 5.935 | 5.063 | 4.279 | 3.580 | 2.962 | 2.423 | 1.961 | 1.572 | 1.255 | 1.007 | 0.825 | 0.708 | 0.653 | 0.658 | 0.721 | 0.839 | 1.012 | 1.237 | 1.513 | 1.836 | 2.207 | 2.623 | 3.082 |
| 98.5 | 5.788 | 4.921 | 4.141 | 3.445 | 2.832 | 2.297 | 1.838 | 1.454 | 1.143 | 0.896 | 0.718 | 0.605 | 0.553 | 0.562 | 0.628 | 0.751 | 0.927 | 1.156 | 1.435 | 1.761 | 2.136 | 2.555 | 3.018 |
| 99.0 | 5.650 | 4.787 | 4.011 | 3.320 | 2.710 | 2.179 | 1.725 | 1.344 | 1.035 | 0.794 | 0.620 | 0.510 | 0.463 | 0.475 | 0.545 | 0.671 | 0.851 | 1.083 | 1.365 | 1.696 | 2.073 | 2.496 | 2.962 |
| 99.5 | 5.522 | 4.662 | 3.891 | 3.203 | 2.597 | 2.071 | 1.620 | 1.243 | 0.937 | 0.701 | 0.530 | 0.424 | 0.380 | 0.396 | 0.469 | 0.599 | 0.782 | 1.018 | 1.303 | 1.637 | 2.018 | 2.444 | 2.915 |
| 100.0 | 5.402 | 4.547 | 3.779 | 3.095 | 2.493 | 1.970 | 1.524 | 1.151 | 0.849 | 0.616 | 0.449 | 0.346 | 0.306 | 0.325 | 0.402 | 0.538 | 0.722 | 0.961 | 1.250 | 1.587 | 1.971 | 2.400 | 2.873 |
| 100.5 | 5.291 | 4.439 | 3.676 | 2.996 | 2.398 | 1.879 | 1.436 | 1.067 | 0.768 | 0.539 | 0.376 | 0.277 | 0.240 | 0.263 | 0.344 | 0.486 | 0.670 | 0.912 | 1.205 | 1.545 | 1.932 | 2.365 | 2.840 |
| 101.0 | 5.188 | 4.341 | 3.581 | 2.905 | 2.311 | 1.796 | 1.357 | 0.991 | 0.696 | 0.471 | 0.311 | 0.216 | 0.182 | 0.209 | 0.293 | 0.433 | 0.626 | 0.870 | 1.167 | 1.511 | 1.901 | 2.337 | 2.815 |
| 101.5 | 5.095 | 4.251 | 3.495 | 2.823 | 2.233 | 1.721 | 1.286 | 0.924 | 0.633 | 0.411 | 0.255 | 0.163 | 0.133 | 0.163 | 0.250 | 0.393 | 0.589 | 0.839 | 1.138 | 1.485 | 1.878 | 2.317 | 2.798 |
| 102.0 | 5.009 | 4.170 | 3.417 | 2.749 | 2.163 | 1.655 | 1.223 | 0.865 | 0.577 | 0.359 | 0.206 | 0.118 | 0.091 | 0.125 | 0.215 | 0.364 | 0.562 | 0.814 | 1.116 | 1.466 | 1.863 | 2.304 | 2.789 |
| 102.5 | 4.933 | 4.097 | 3.348 | 2.684 | 2.101 | 1.597 | 1.169 | 0.814 | 0.530 | 0.316 | 0.166 | 0.081 | 0.058 | 0.096 | 0.189 | 0.345 | 0.542 | 0.797 | 1.102 | 1.455 | 1.858 | 2.305 | 2.797 |
| 103.0 | 4.864 | 4.032 | 3.288 | 2.627 | 2.048 | 1.547 | 1.122 | 0.771 | 0.491 | 0.279 | 0.134 | 0.052 | 0.033 | 0.072 | 0.170 | 0.323 | 0.529 | 0.784 | 1.095 | 1.452 | 1.857 | 2.309 | 2.793 |
| 103.5 | 4.804 | 3.976 | 3.235 | 2.578 | 2.002 | 1.505 | 1.084 | 0.737 | 0.460 | 0.252 | 0.110 | 0.031 | 0.015 | 0.058 | 0.159 | 0.315 | 0.525 | 0.786 | 1.097 | 1.457 | 1.863 | 2.313 | 2.807 |
| 104.0 | 4.753 | 3.928 | 3.191 | 2.537 | 1.965 | 1.472 | 1.054 | 0.710 | 0.437 | 0.232 | 0.093 | 0.018 | 0.005 | 0.052 | 0.155 | 0.315 | 0.528 | 0.792 | 1.107 | 1.469 | 1.878 | 2.331 | 2.828 |
| 104.5 | 4.709 | 3.888 | 3.155 | 2.505 | 1.936 | 1.446 | 1.032 | 0.692 | 0.422 | 0.220 | 0.085 | 0.013 | 0.000 | 0.053 | 0.160 | 0.322 | 0.538 | 0.806 | 1.123 | 1.489 | 1.900 | 2.357 | 2.856 |
| 105.0 | 4.674 | 3.857 | 3.128 | 2.480 | 1.915 | 1.429 | 1.018 | 0.681 | 0.414 | 0.214 | 0.084 | 0.016 | 0.009 | 0.062 | 0.172 | 0.337 | 0.557 | 0.827 | 1.148 | 1.516 | 1.930 | 2.390 | 2.892 |
| 105.5 | 4.647 | 3.833 | 3.106 | 2.464 | 1.902 | 1.419 | 1.012 | 0.678 | 0.415 | 0.220 | 0.091 | 0.026 | 0.022 | 0.078 | 0.191 | 0.360 | 0.582 | 0.856 | 1.179 | 1.550 | 1.968 | 2.430 | 2.935 |
| 106.0 | 4.627 | 3.817 | 3.094 | 2.455 | 1.897 | 1.417 | 1.013 | 0.683 | 0.423 | 0.231 | 0.105 | 0.044 | 0.043 | 0.102 | 0.219 | 0.390 | 0.615 | 0.892 | 1.218 | 1.592 | 2.013 | 2.477 | 2.985 |
| 106.5 | 4.616 | 3.809 | 3.090 | 2.454 | 1.899 | 1.423 | 1.022 | 0.695 | 0.438 | 0.250 | 0.128 | 0.069 | 0.072 | 0.134 | 0.253 | 0.428 | 0.656 | 0.935 | 1.264 | 1.641 | 2.064 | 2.532 | 3.043 |
| 107.0 | 4.612 | 3.809 | 3.093 | 2.461 | 1.909 | 1.436 | 1.039 | 0.715 | 0.462 | 0.276 | 0.157 | 0.102 | 0.107 | 0.173 | 0.294 | 0.474 | 0.706 | 0.986 | 1.318 | 1.698 | 2.124 | 2.594 | 3.107 |
| 107.5 | 4.616 | 3.817 | 3.104 | 2.475 | 1.927 | 1.457 | 1.063 | 0.743 | 0.492 | 0.310 | 0.194 | 0.142 | 0.151 | 0.219 | 0.344 | 0.525 | 0.758 | 1.044 | 1.379 | 1.761 | 2.190 | 2.663 | 3.179 |
| 108.0 | 4.628 | 3.832 | 3.122 | 2.497 | 1.952 | 1.486 | 1.095 | 0.778 | 0.531 | 0.352 | 0.239 | 0.189 | 0.201 | 0.272 | 0.400 | 0.584 | 0.821 | 1.109 | 1.446 | 1.832 | 2.263 | 2.739 | 3.257 |
| 108.5 | 4.647 | 3.855 | 3.149 | 2.526 | 1.985 | 1.522 | 1.134 | 0.820 | 0.576 | 0.400 | 0.290 | 0.244 | 0.259 | 0.333 | 0.464 | 0.650 | 0.890 | 1.181 | 1.521 | 1.909 | 2.343 | 2.822 | 3.343 |
| 109.0 | 4.674 | 3.885 | 3.182 | 2.563 | 2.025 | 1.565 | 1.181 | 0.869 | 0.629 | 0.455 | 0.349 | 0.306 | 0.323 | 0.400 | 0.534 | 0.724 | 0.966 | 1.260 | 1.603 | 1.994 | 2.430 | 2.911 | 3.435 |
| 109.5 | 4.709 | 3.922 | 3.223 | 2.607 | 2.072 | 1.616 | 1.234 | 0.926 | 0.689 | 0.519 | 0.415 | 0.374 | 0.395 | 0.475 | 0.612 | 0.804 | 1.049 | 1.346 | 1.692 | 2.085 | 2.524 | 3.008 | 3.534 |
| 110.0 | 4.750 | 3.967 | 3.271 | 2.659 | 2.127 | 1.673 | 1.295 | 0.990 | 0.756 | 0.589 | 0.488 | 0.450 | 0.474 | 0.557 | 0.697 | 0.891 | 1.139 | 1.438 | 1.787 | 2.183 | 2.625 | 3.111 | 3.640 |
| 110.5 | 4.799 | 4.020 | 3.327 | 2.717 | 2.189 | 1.738 | 1.363 | 1.061 | 0.830 | 0.666 | 0.568 | 0.533 | 0.560 | 0.645 | 0.788 | 0.988 | 1.236 | 1.538 | 1.889 | 2.288 | 2.733 | 3.221 | 3.753 |
| 111.0 | 4.855 | 4.079 | 3.389 | 2.783 | 2.257 | 1.810 | 1.438 | 1.139 | 0.910 | 0.750 | 0.655 | 0.623 | 0.652 | 0.741 | 0.886 | 1.092 | 1.340 | 1.644 | 1.998 | 2.399 | 2.847 | 3.338 | 3.872 |
| 111.5 | 4.918 | 4.145 | 3.459 | 2.855 | 2.333 | 1.889 | 1.520 | 1.224 | 0.998 | 0.841 | 0.748 | 0.719 | 0.752 | 0.843 | 0.991 | 1.194 | 1.450 | 1.757 | 2.114 | 2.518 | 2.967 | 3.461 | 3.997 |
| 112.0 | 4.988 | 4.218 | 3.535 | 2.935 | 2.416 | 1.975 | 1.609 | 1.316 | 1.093 | 0.938 | 0.849 | 0.823 | 0.858 | 0.952 | 1.103 | 1.308 | 1.567 | 1.877 | 2.236 | 2.642 | 3.094 | 3.591 | 4.132 |
| 112.5 | 5.066 | 4.299 | 3.618 | 3.021 | 2.505 | 2.067 | 1.704 | 1.414 | 1.194 | 1.042 | 0.956 | 0.933 | 0.970 | 1.067 | 1.221 | 1.429 | 1.690 | 2.003 | 2.364 | 2.773 | 3.228 | 3.727 | 4.268 |
| 113.0 | 5.149 | 4.386 | 3.708 | 3.115 | 2.602 | 2.166 | 1.806 | 1.519 | 1.302 | 1.153 | 1.069 | 1.056 | 1.096 | 1.189 | 1.345 | 1.556 | 1.820 | 2.135 | 2.499 | 2.911 | 3.368 | 3.869 | 4.413 |
| 113.5 | 5.240 | 4.480 | 3.805 | 3.215 | 2.704 | 2.272 | 1.915 | 1.631 | 1.417 | 1.270 | 1.190 | 1.172 | 1.215 | 1.317 | 1.476 | 1.690 | 1.956 | 2.274 | 2.641 | 3.055 | 3.514 | 4.018 | 4.564 |
| 114.0 | 5.338 | 4.580 | 3.909 | 3.321 | 2.814 | 2.384 | 2.030 | 1.749 | 1.538 | 1.394 | 1.316 | 1.301 | 1.347 | 1.452 | 1.614 | 1.830 | 2.099 | 2.419 | 2.788 | 3.205 | 3.667 | 4.173 | 4.721 |
| 114.5 | 5.441 | 4.687 | 4.019 | 3.434 | 2.930 | 2.503 | 2.152 | 1.878 | 1.665 | 1.524 | 1.449 | 1.437 | 1.485 | 1.593 | 1.757 | 1.976 | 2.248 | 2.570 | 2.942 | 3.361 | 3.825 | 4.333 | 4.884 |
| 115.0 | 5.552 | 4.800 | 4.135 | 3.553 | 3.052 | 2.629 | 2.280 | 2.004 | 1.799 | 1.661 | 1.588 | 1.579 | 1.630 | 1.740 | 1.907 | 2.128 | 2.403 | 2.728 | 3.102 | 3.523 | 3.990 | 4.500 | 5.053 |
| 115.5 | 5.669 | 4.920 | 4.258 | 3.679 | 3.181 | 2.760 | 2.414 | 2.142 | 1.939 | 1.803 | 1.734 | 1.727 | 1.781 | 1.893 | 2.063 | 2.287 | 2.563 | 2.891 | 3.267 | 3.691 | 4.160 | 4.673 | 5.229 |
| 116.0 | 5.792 | 5.046 | 4.387 | 3.811 | 3.315 | 2.898 | 2.555 | 2.285 | 2.085 | 1.952 | 1.885 | 1.881 | 1.937 | 2.053 | 2.225 | 2.451 | 2.730 | 3.060 | 3.439 | 3.865 | 4.337 | 4.852 | 5.410 |
| 116.5 | 5.921 | 5.179 | 4.522 | 3.949 | 3.456 | 3.041 | 2.702 | 2.434 | 2.237 | 2.107 | 2.042 | 2.041 | 2.100 | 2.218 | 2.392 | 2.621 | 2.903 | 3.235 | 3.617 | 4.045 | 4.519 | 5.037 | 5.597 |

How flexible is the water molecule structure? Analysis of crystal structures and the potential energy surface (https://doi.org/10.1039/C9CP07042G)

# Parabola, paraboloid

1 proměnná

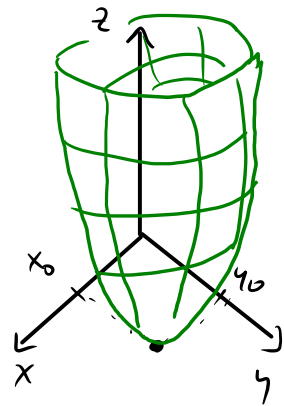
$y = (x - x_0)^2$




parabola se vrcholem v $x_0$

2 proměnné

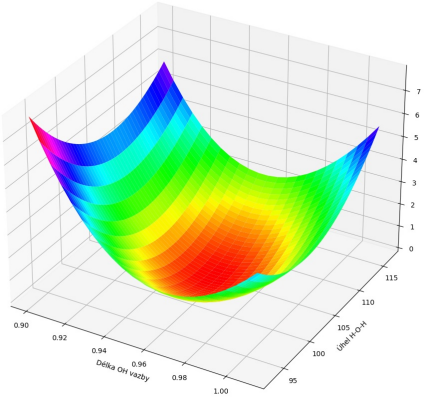
$z = (x - x_0)^2 + (y - y_0)^2$



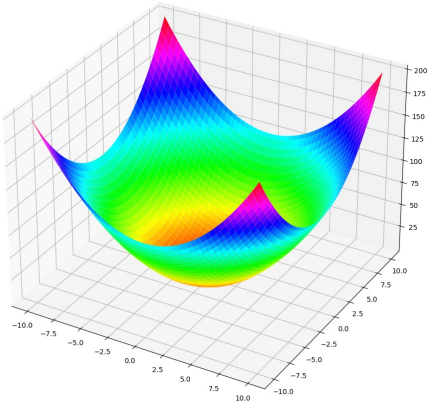

paraboloid s vrcholem v $(x_0, y_0)$

# Molekula vody III

Změna potenciální energie $\Delta E$
molekuly vody




Paraboloid $z = x^2 + y^2$



# Optimalizace ve více proměnných

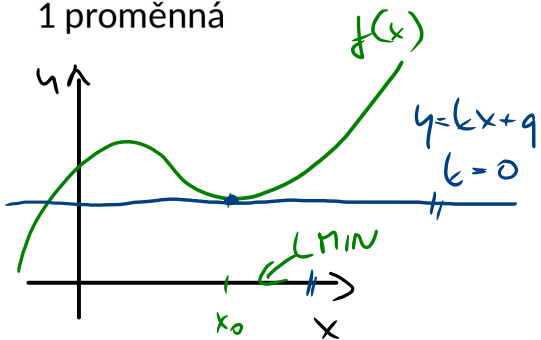
- často výrazně větší počet proměnných (= parametrů modelu)
- příklad pro molekuly: lokální minimum ~ stabilní konformace

Způsoby řešení

- 2 proměnné, jednoduchá funkce ⇒ ANALYTICKY
- více proměnných nebo složitější funkce ⇒ NUMERICKY (POČÍTAČ)

# Extrémy funkcí jedné a dvou proměnných

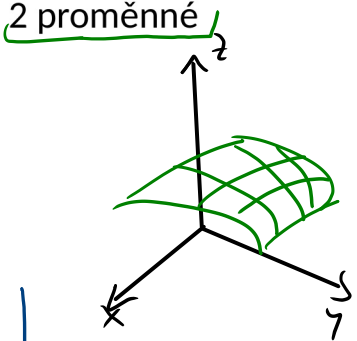
1 proměnná




$k = f'(x_0) = 0$

$\frac{df(x)}{dx} = 0$ "dle x"

2 proměnné




↳ 2 DERIVACE PARCIÁLNÍ

# Parciální derivace

$z = f(x,y)$

$\frac{\partial z}{\partial x}$ = parc. der. z podle x $\Rightarrow$ jak se mění z ve směru osy x

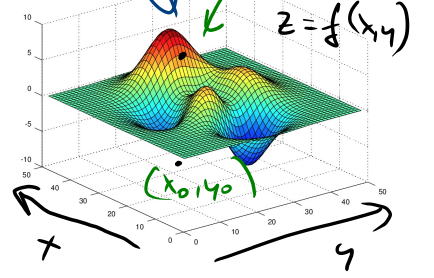
$\frac{\partial z}{\partial y}$ = ... podle y

$\partial \neq \delta$

parc. der. — delta

$\frac{\partial z}{\partial x} = \frac{\partial f(x,y)}{\partial x} = \frac{\partial}{\partial x} f(x,y)$

$\left.\frac{\partial z}{\partial y}\right|_{(x_0,y_0)} < 0$ $\left.\frac{\partial z}{\partial x}\right|_{(x_0,y_0)} > 0$



# Výpočet parciálních derivací

- Při derivaci dle konkrétní proměnné považuji ostatní proměnné za konstanty.
- Platí všechna ostatní pravidla z derivací funkcí jedné proměnné.

Př.: $f(x,y) = \sin(xy^2)$

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}\left(\sin(xy^2)\right) = \cos(xy^2)\cdot\frac{\partial}{\partial x}(xy^2) = \cos(xy^2)\cdot y^2$$

$g(x,y) = x^2 + 3y$

$$\frac{\partial g}{\partial y} = \frac{\partial}{\partial y}(x^2+3y) = 3$$

$h(x,y) = e^x$

$$\frac{\partial h}{\partial x} = e^x \qquad \frac{\partial h}{\partial y} = 0$$

# Výpočty druhých parciálních derivací

$$\frac{\partial^2 f(x,y)}{\partial x^2}, \quad \frac{\partial^2 f(x,y)}{\partial y^2}, \quad \frac{\partial^2 f(x,y)}{\partial x \partial y} = \frac{\partial^2 f(x,y)}{\partial y \partial x}$$

↳ NEZÁLEŽÍ NA POŘADÍ DERIVACÍ

**Př:**

$$\frac{\partial^2}{\partial x \partial y}(x \cdot \sin y) = \frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}(x \sin y)\right) = \frac{\partial}{\partial y}(\sin y) = \cos y$$

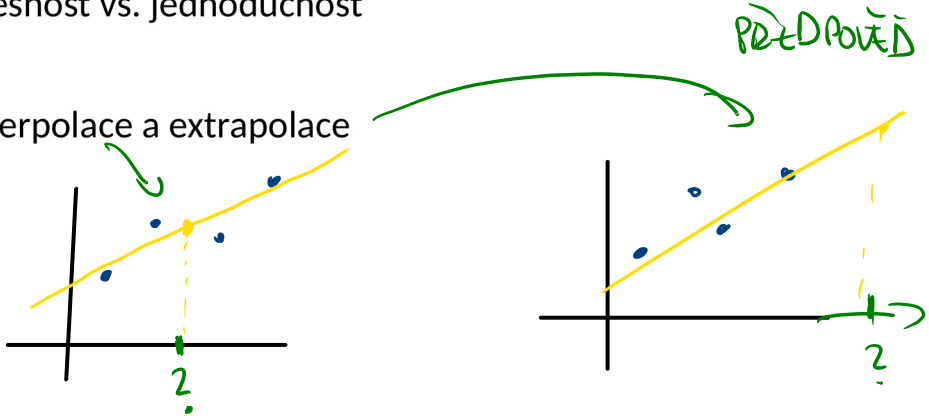
$$\frac{\partial^2}{\partial y \partial x}(x \cdot \sin y) = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial y}(x \cdot \sin y)\right) = \frac{\partial}{\partial x}(x \cdot \cos y) = \cos y$$

# Modely

Matematický model = formální popis nějakého systému.

Přesnost vs. jednoduchost

Interpolace a extrapolace



# Cena lístku v divadle

c ... cena lístku

p(c) ... počet diváků při ceně c

$p(50) = 4000$

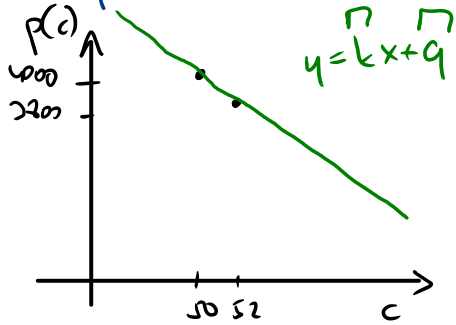
$p(52) = 3800$

$4000 = k \cdot 50 + q$

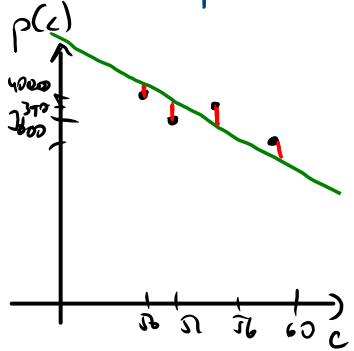
$3800 = k \cdot 52 + q$

$p(56) = 3900$

$p(60) = 3700$




$y = kx + q$



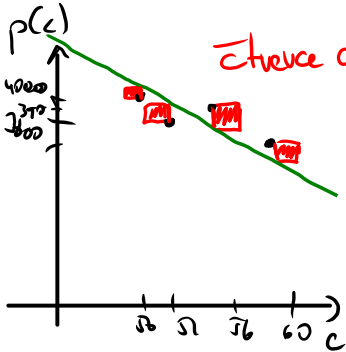

CÍL: minimalizace chyb

# Metoda nejmenších čtverců I

LINEÁRNÍ MODEL

$M(c) = kc + q$

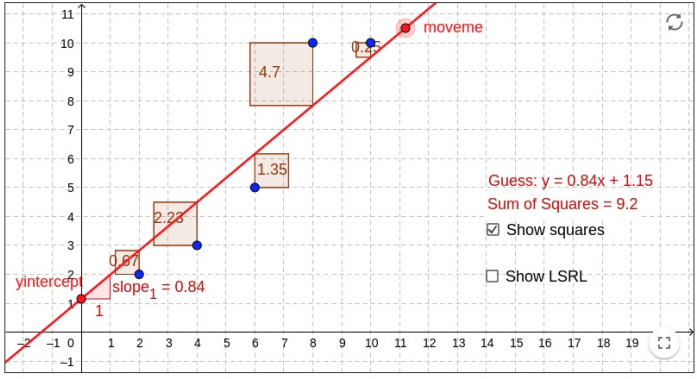
↳ predikovaná hodnota účasti při ceně $c$



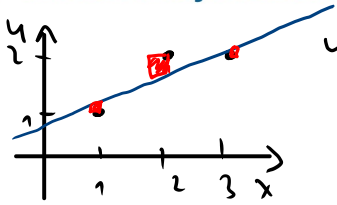

$$\min_{k,q} \left[ \left(M(50) - 4000\right)^2 + \left(M(52) - 3800\right)^2 + \left(M(56) - 3900\right)^2 + \left(M(60) - 3700\right)^2 \right]$$

# Metoda nejmenších čtverců II

https://www.geogebra.org/m/JsFmFEg6



# Metoda nejmenších čtverců III – příklad




$y = kx + q$

$$\left.\begin{aligned} 1 &= 1k + q \\ 2 &= 2k + q \\ 2 &= 3k + q \end{aligned}\right\}$$ soustava nemá řešení!

$$E(k,q) = ((k1+q)-1)^2 + ((k2+q)-2)^2 + ((k3+q)-2)^2$$

$$\frac{\partial E(k,q)}{\partial k} = 2(k+q-1) + 2(2k+q-2)\cdot 2 + 2(3k+q-2)\cdot 3 = 28k + 12q - 22$$

$$\frac{\partial E(k,q)}{\partial q} = 2(k+q-1) + 2(2k+q-2) + 2(3k+q-2) = 12k + 6q - 10$$

# Metoda nejmenších čtverců IV – příklad

$$28k + 12q = 22$$
$$12k + 6q = 10$$

$$\left[\begin{array}{cc|c} 14 & 6 & 11 \\ 6 & 3 & 5 \end{array}\right] \sim \left[\begin{array}{cc|c} 2 & 0 & 1 \\ 6 & 3 & 5 \end{array}\right] \sim \left[\begin{array}{cc|c} 2 & 0 & 1 \\ 0 & 3 & 2 \end{array}\right]$$

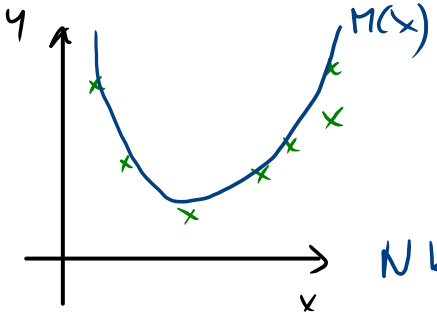
$2k = 1 \Rightarrow k = 1/2$

$3q = 2 \quad q = 2/3$

$y = 1/2\,x + 2/3$

# Metoda nejmenších čtverců V – zobecnění

Obecně různé modely: LINEÁRNÍ, KVADRATICKÝ, EXP, LOG




$$M(x) = ax^2 + bx + c$$

↳ 3 parametry
↳ 3 parc. derivace
↳ 3 rovnice o 3 neznámých

N bodů $(x_i, y_i)$

$$\min_{a,b,c} \sum_{i=1}^{N} \left( M(x_i) - y_i \right)^2$$

$y_i$ … skutečná hodnota

$M(x_i)$ … modelem predikovaná hodnota

$$M(x_i) = ax_i^2 + bx_i + c$$

# Výběr modelu